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=> b hcap
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FILE COVERS 1907 - 1 May 2008  VOL 148 ISS 18
FILE LAST UPDATED: 30 Apr 2008  (20080430/ED)

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 substance identification.

=> d bib abs hitstr l27 tot
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L27 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:371235 HCAPLUS
DN 142:412276
TI High-purity piperazine pyrophosphate and method for producing same
IN Kimura, Ryoji; Murase, Hisashi; Nagahama, Masaru; Kamimoto, Tetsuo; Nakano, Shinji
PA Asahi Denka Co., Ltd., Japan
SO PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO--2005037806	A1	20050428	2004WO-JP0012379	20040827
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP--2005120021	A	20050512	2003JP-000356864	20031016
EP-----1674459	A1	20060628	2004EP-000772335	20040827
R: DE, FR, GB				
CN-----1845913	A	20061011	2004CN-080025664	20040827
IN-2005KN02679	A	20061103	2005IN-KN0002679	20051222
US-20060167256	A1	20060727	2006US-000563478	20060105 <--
PRAI 2003JP-000356864	A	20031016		
2004WO-JP0012379	W	20040827		

AB Piperazine diphosphate (I) is dehydrated to prepare piperazine pyrophosphate (II) for fireproofing agents for plastics. Thus, I was extruded to give II and added to a polypropylene composition
IT 66034-17-1P, Piperazine monopyrophosphate
RL: IMF (Industrial manufacture); MOA (Modifier or additive use); PREP (Preparation); USES (Uses)
(high-purity piperazine pyrophosphate for fireproofing agents for plastics)
RN 66034-17-1 HCAPLUS
CN Diphosphoric acid, compd. with piperazine (1:1) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

CM 2

CRN 110-85-0
CMF C4 H10 N2

L27 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
IT 52978-33-3, Piperazine diphosphate
RL: RCT (Reactant); RACT (Reactant or reagent)
(high-purity piperazine pyrophosphate for fireproofing agents for plastics)
RN 52978-33-3 HCAPLUS
CN Piperazine, phosphate (1:2) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
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=> b uspatall
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FILE 'USPATOLD' ENTERED AT 11:22:03 ON 01 MAY 2008
CA INDEXING COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

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CA INDEXING COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs hitstr l17 tot
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L17 ANSWER 1 OF 9 USPATFULL on STN
AN 2008:33694 USPATFULL
TI Compositions and methods for improved planarization of copper utilizing inorganic oxide abrasive
IN Thomas, Terence M., Newark, DE, UNITED STATES
PI US-20080029126 A1 20080207
AI 2006US-000500072 A1 20060807 (11)
DT Utility
FS APPLICATION
LREP ROHM AND HAAS ELECTRONIC MATERIALS, CMP HOLDINGS, INC., 451 BELLEVUE ROAD, NEWARK, DE, 19713, US
CLMN Number of Claims: 10
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 563
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention provides an aqueous composition useful for polishing copper on a semiconductor wafer at a down force pressure of at least less than 20.68 kPa, comprising by weight percent oxidizer, 0.001 to 5 inhibitor for a nonferrous metal, complexing agent for the nonferrous metal, 0.01 to 5 carboxylic acid polymer, 0.01 to 5 modified cellulose, 0.001 to 10 phosphorus-containing compound and 0.001 to 10 boehmite abrasive, wherein the boehmite increases the planarization rate of the copper.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 14538-56-8, Piperazine phosphate 52492-62-3, Piperazine diphosphate
(in polishing compns.; chemical-mech. polishing compns. for improved planarization of copper using boehmite abrasives)
RN 14538-56-8 USPATFULL
CN Piperazine, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

RN 52492-62-3 USPATFULL
CN Diphosphoric acid, compd. with piperazine (1:?) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

L17 ANSWER 1 OF 9 USPATFULL on STN (Continued)

CM 2

CRN 110-85-0
CMF C4 H10 N2

L17 ANSWER 2 OF 9 USPATFULL on STN
AN 2007:201510 USPATFULL
TI Flame retardant composition with improved fluidity, flame retardant resin composition and molded products
IN Murase, Hisashi, Saitama, JAPAN
Nagahama, Masaru, Saitama, JAPAN
Yoshikawa, Kenichi, Saitama, JAPAN
Tanaka, Yuki, Saitama, JAPAN
Kaneda, Takayoshi, Saitama, JAPAN
Yamaki, Akihiro, Saitama, JAPAN
PA AKEKA CORPORATION, TOKYO, JAPAN, JAPAN, 116-0012 (non-U.S. corporation)
PI US-20070176154 A1 20070802
AI 2005US-000590350 A1 20050222 (10)
2005WO-JP0003260 20050222
20060823 PCT 371 date
PRAI 2004JP-000048664 20040224
DT Utility
FS APPLICATION
LREP Millen White Zelano & Branigan, Arlington Courthouse Plaza I, 2200 Clarendon Boulevard Suite 1400, Arlington, VA, 22201, US
CLMN Number of Claims: 7
ECL Exemplary Claim: 1
DRWN 1 Drawing Page(s)
LN.CNT 814
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention provides a flame retardant composition comprising 1-99 weight parts of a salt of piperazine and an inorganic compound selected from among piperazine phosphate, piperazine pyrophosphate and piperazine polyphosphate, or a mixture of two or more of these piperazine salts (ingredient (A)), 99-1 weight parts of a salt of melamine and an inorganic compound selected from among melamine phosphate, melamine pyrophosphate and melamine polyphosphate, or a mixture of two or more of these melamine salts (ingredient (B)) (wherein, the sum of ingredient (A) and ingredient (B) is 100 weight parts), 0-50 weight parts of an arbitrary ingredient (ingredient (C)), and 0.01-20 weight parts of a silicone oil having a viscosity at 25° C. of 5000 mm.sup.2/s (ingredient (D)) which is added thereto. This flame retardant not only has superior flame retarding properties, but also has enhanced powder properties and anti-hygroscopic properties, and when it is added to a resin, there is little change of electrical resistance.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 1951-97-9 66034-17-1, 1:1 Piperazine pyrophosphate
(flame-retardant compns. containing phosphates of piperazine and melamine treated with silicone oil for enhanced fluidity)
RN 1951-97-9 USPATFULL
CN Piperazine, phosphate (8CI, 9CI) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

RN 66034-17-1 USPATFULL

L17 ANSWER 2 OF 9 USPATFULL on STN (Continued)
CN Diphosphoric acid, compd. with piperazine (1:1) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

CM 2

CRN 110-85-0
CMF C4 H10 N2

L17 ANSWER 3 OF 9 USPATFULL on STN
AN 2007:140258 USPATFULL
TI WOOD SCREWS CAPABLE OF CUTTING WOOD
IN LIN, Chao Wei, Tainan County, TAIWAN, PROVINCE OF CHINA
PA KWANTAX RESEARCH INC., TAINAN COUNTY, TAIWAN, PROVINCE OF CHINA, 71848 (non-U.S. corporation)
PI US-20070122249 A1 20070531
AI 2006US-000563478 A1 20061127 (11)
PRAI 2005TW-094142072 20051130
DT Utility
FS APPLICATION
LREP LOWE HAUPTMAN BERNER, LLP, 1700 DIAGONAL ROAD, SUITE 300, ALEXANDRIA, VA, 22314, US
CLMN Number of Claims: 16
ECL Exemplary Claim: 1
DRWN 5 Drawing Page(s)
LN.CNT 265
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A wood screw includes a head, a shank, an engagement thread, at least one parallel thread and at least one guiding thread. The head is for receiving a fastening tool. The shank extends from the head and includes a parallel shank portion, a tapered portion formed at the tip of the parallel shank portion and a pointed end formed at the tip of the tapered portion. The engagement thread is formed on the parallel shank portion. The at least one parallel thread is formed on the tapered portion. Then at least one guiding thread is formed on the tapered portion and between the parallel thread and the engagement thread.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 66034-17-1P, Piperazine monopyrophosphate
(high-purity piperazine pyrophosphate for fireproofing agents for plastics)
RN 66034-17-1 USPATFULL
CN Diphosphoric acid, compd. with piperazine (1:1) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

CM 2

CRN 110-85-0
CMF C4 H10 N2

IT 52978-33-3, Piperazine diphosphate
(high-purity piperazine pyrophosphate for fireproofing agents for plastics)
RN 52978-33-3 USPATFULL
CN Piperazine, phosphate (1:2) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

L17 ANSWER 3 OF 9 USPATFULL on STN (Continued)

CM 2

CRN 110-85-0
CMF C4 H10 N2

L17 ANSWER 4 OF 9 USPATFULL on STN
AN 2006:196499 USPATFULL
TI High purity piperazine pyrophosphate and process of producing same
IN Kimura, Ryoji, Saitama, JAPAN
Nagahama, Masaru, Saitama, JAPAN
Kamimoto, Tetsuo, Saitama, JAPAN
Nakano, Shinji, Saitama, JAPAN
PI US-20060167256 A1 20060727
AI 2004US-000563478 A1 20040827 (10)
2004WO-JP0012379 20040827
20060105 PCT 371 date
PRAI 2003JP-000356864 20031016
DT Utility
FS APPLICATION
LREP YOUNG & THOMPSON, 745 SOUTH 23RD STREET, 2ND FLOOR, ARLINGTON, VA, 22202, US
CLMN Number of Claims: 2
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 390
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention provides piperazine pyrophosphate represented by chemical formula (I) which has a sodium content of 10 ppm or lower and a process of producing the same. The piperazine pyrophosphate has high purity and provides a flame retardant composition exhibiting excellent flame retardancy. The process includes dehydration condensation of piperazine diphosphate and is able to produce the piperazine pyrophosphate at low cost. ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 66034-17-1P, Piperazine monopyrophosphate
(high-purity piperazine pyrophosphate for fireproofing agents for plastics)
RN 66034-17-1 USPATFULL
CN Diphosphoric acid, compd. with piperazine (1:1) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

CM 2

CRN 110-85-0
CMF C4 H10 N2

IT 52978-33-3, Piperazine diphosphate
(high-purity piperazine pyrophosphate for fireproofing agents for plastics)
RN 52978-33-3 USPATFULL
CN Piperazine, phosphate (1:2) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

L17 ANSWER 4 OF 9 USPATFULL on STN (Continued)

CM 2

CRN 110-85-0
CMF C4 H10 N2

L17 ANSWER 5 OF 9 USPATFULL on STN
AN 2005:224513 USPATFULL
TI MULTI-STEP POLISHING SOLUTION FOR CHEMICAL MECHANICAL PLANARIZATION
IN Liu, Zhendong, Newark, DE, UNITED STATES
Quanci, John, Haddonfield, NJ, UNITED STATES
Schmidt, Robert E., Bear, DE, UNITED STATES
Thomas, Terence M., Newark, DE, UNITED STATES
PI US-20050194357 A1 20050908
US-----6971945 B2 20051206
AI 2004US-000785362 A1 20040223 (10)
DT Utility
FS APPLICATION
LREP Rohm and Haas, Electronic Materials CMP Holdings, Inc., Suite 1300, 1105 North Market Street, Wilmington, DE, 19899, US
CLMN Number of Claims: 10
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 648
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention provides a multi-step aqueous composition useful for polishing a tantalum barrier material and copper from a semiconductor wafer, comprising by weight percent 0.1 to 30 oxidizer, 0.01 to 3 inorganic salt or acid, 0.01 to 4 inhibitor, 0.1 to 30 abrasive, 0 to 15 complexing agent and balance water, wherein the aqueous composition has a pH between 1.5 to 6.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 14538-56-8, Piperazine phosphate 52492-62-3, Piperazine pyrophosphate
(component of polishing paste; multi-step polishing solution for chemical mech. planarization of metal films on semiconductor wafer)
RN 14538-56-8 USPATFULL
CN Piperazine, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

RN 52492-62-3 USPATFULL
CN Diphosphoric acid, compd. with piperazine (1:?) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

L17 ANSWER 5 OF 9 USPATFULL on STN (Continued)

CM 2

CRN 110-85-0
CMF C4 H10 N2

L17 ANSWER 6 OF 9 USPATFULL on STN
AN 2005:158463 USPATFULL
TI Compositions and methods for low downforce pressure polishing of copper
IN Goldberg, Wendy B., Sequim, WA, UNITED STATES
Kelley, Francis J., Bear, DE, UNITED STATES
Quanci, John, Haddonfield, NJ, UNITED STATES
So, Joseph K., Newark, DE, UNITED STATES
Thomas, Terence M., Newark, DE, UNITED STATES
Wang, Hongyu, Wilmington, DE, UNITED STATES
PI US-20050136671 A1 20050623
AI 2003US-000742961 A1 20031222 (10)
DT Utility
FS APPLICATION
LREP Rodel Holdings, Inc., Suite 1300, 1105 North Market Street, Wilmington, DE, 19899, US
CLMN Number of Claims: 10
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 499
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention provides an aqueous composition useful for polishing copper on a semiconductor wafer at a down force pressure of at least less than 20.68 kPa, comprising by weight percent 1 to 15 oxidizer, 0.1 to 1 inhibitor for a nonferrous metal, 0.05 to 3 complexing agent for the nonferrous metal, 0.01 to 5 carboxylic acid polymer, 0.01 to 5 modified cellulose, 0.05 to 10 phosphorus-containing compound and 0 to 10 abrasive, wherein the phosphorus-containing compound increases removal of the copper.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 14538-56-8, Piperazine phosphate 52492-62-3, Piperazine pyrophosphate
(in composition for low down-force pressure polishing of copper on semiconductor wafers)
RN 14538-56-8 USPATFULL
CN Piperazine, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

RN 52492-62-3 USPATFULL
CN Diphosphoric acid, compd. with piperazine (1:?) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

L17 ANSWER 6 OF 9 USPATFULL on STN (Continued)

CM 2

CRN 110-85-0
CMF C4 H10 N2

L17 ANSWER 7 OF 9 USPATFULL on STN
AN 2003:127785 USPATFULL
TI Flame-retardant resin composition
IN Kimura, Ryoji, Saitama-shi, JAPAN
Matsuzaka, Nobuo, Saitama-shi, JAPAN
Nakajima, Toshio, Saitama-shi, JAPAN
Yamaki, Akihiro, Saitama-shi, JAPAN
Murase, Hisashi, Saitama-shi, JAPAN
PA ASAHI DENKA KOGYO KABUSHIKI KAISHA, Tokyo, JAPAN (non-U.S. corporation)
PI US-20030088000 A1 20030508
AI 2002US-000186631 A1 20020702 (10)
PRAI 2001JP-000216397 20010717
DT Utility
FS APPLICATION
LREP YOUNG & THOMPSON, 745 SOUTH 23RD STREET 2ND FLOOR, ARLINGTON, VA, 22202
CLMN Number of Claims: 13
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 597
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A flame-retardant resin composition comprising (A) a synthetic resin, (B) (b1) a specific phosphoric acid salt or (b2) a combination of specific phosphoric acid salts, and (C) an anti-dripping agent.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 14538-56-8, Piperazine phosphate 52492-62-3, Piperazine pyrophosphate
(fireproofing agent; fire-resistant resin compns. containing phosphoric acid salts)
RN 14538-56-8 USPATFULL
CN Piperazine, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

RN 52492-62-3 USPATFULL
CN Diphosphoric acid, compd. with piperazine (1:?) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

L17 ANSWER 7 OF 9 USPATFULL on STN (Continued)

CM 2

CRN 110-85-0
CMF C4 H10 N2

L17 ANSWER 8 OF 9 USPATOLD on STN
AN 1974:67280 USPATOLD
TI PIPERAZINE PHOSPHATES AS FIRE RETARDANTS FOR ORGANIC POLYMERS
IN ROWTON R
PA JEFFERSON CHEMICAL COMPANY, INC.
PI US-----3810850 A 19740514
AI 1973US-000321794 19730101
PRAI 1973US-000321794 19730108
DT Utility
FS GRANTED
EXNAM Primary Examiner: CZAJA, DONALD E; Assistant Examiner: IVY, C WARREN
LN.CNT 982
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 14538-56-8 52492-62-3 52978-33-3
(fireproofing agents, for resins)
RN 14538-56-8 USPATOLD
CN Piperazine, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

RN 52492-62-3 USPATOLD
CN Diphosphoric acid, compd. with piperazine (1:?) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

CM 2

CRN 110-85-0
CMF C4 H10 N2

RN 52978-33-3 USPATOLD

L17 ANSWER 8 OF 9 USPATOLD on STN (Continued)
CN Piperazine, phosphate (1:2) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

L17 ANSWER 9 OF 9 USPAT2 on STN
AN 2005:224513 USPAT2
TI Multi-step polishing solution for chemical mechanical planarization
IN Liu, Zhendong, Newark, DE, UNITED STATES
Quanci, John, Haddonfield, NJ, UNITED STATES
Schmidt, Robert E., Bear, DE, UNITED STATES
Thomas, Terence M., Newark, DE, UNITED STATES
PA Rohm and Haas Electronic Materials CMP Holdings, Inc., Wilmington, DE, UNITED STATES (U.S. corporation)
PI US-----6971945 B2 20051206
AI 2004US-000785362 20040223 (10)
DT Utility
FS GRANTED
EXNAM Primary Examiner: Wilson, Lee D.; Assistant Examiner: Ojini, Anthony
LREP Oh, Edwin
CLMN Number of Claims: 10
ECL Exemplary Claim: 7
DRWN No Drawings
LN.CNT 648
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention provides a multi-step aqueous composition useful for polishing a tantalum barrier material and copper from a semiconductor wafer, comprising by weight percent 0.1 to 30 oxidizer, 0.01 to 3 inorganic salt or acid, 0.01 to 4 inhibitor, 0.1 to 30 abrasive, 0 to 15 complexing agent and balance water, wherein the aqueous composition has a pH between 1.5 to 6.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 14538-56-8, Piperazine phosphate 52492-62-3, Piperazine pyrophosphate
(component of polishing paste; multi-step polishing solution for chemical mech. planarization of metal films on semiconductor wafer)
RN 14538-56-8 USPAT2
CN Piperazine, phosphate (1:1) (CA INDEX NAME)

CM 1

CRN 7664-38-2
CMF H3 O4 P

CM 2

CRN 110-85-0
CMF C4 H10 N2

RN 52492-62-3 USPAT2
CN Diphosphoric acid, compd. with piperazine (1:?) (CA INDEX NAME)

CM 1

CRN 2466-09-3
CMF H4 O7 P2

L17 ANSWER 9 OF 9 USPAT2 on STN (Continued)

CM 2

CRN 110-85-0
CMF C4 H10 N2

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26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 26 Apr 2008 VOL 148 ISS 18

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provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.


L22             STR
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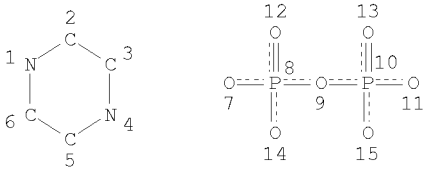


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  15

STEREO ATTRIBUTES: NONE
L25          38 SEA FILE=CASREACT SSS FUL L22 (   371 REACTIONS)

100.0% DONE    1269 VERIFIED     371 HIT RXNS                     38 DOCS
SEARCH TIME: 00.00.01
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L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN

AN 140:423568 CASREACT

TI Anti-calmodulin acridone derivatives modulate vinblastine resistance in multidrug resistant (MDR) cancer cells

AU Hegde, Ravi; Thimmaiah, Padma; Yerigeri, Mayur C.; Krishnegowda, Gowdahalli; Thimmaiah, Kuntebommanahalli N.; Houghton, Peter J.

CS Department of Studies in Chemistry, University of Mysore, Mysore, 570006, India

SO European Journal of Medicinal Chemistry (2004), 39(2), 161-177
CODEN: EJMCA5; ISSN: 0223-5234

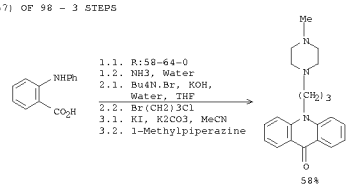
PB Elsevier Science Ltd.

DT Journal

LA English

AB Multidrug resistance (MDR) is one of the main obstacles limiting the efficacy of chemotherapy treatment of tumors. 10-Acridone and its 4-methoxy derivative were prepared by the Ullmann reaction followed by cyclization and N-alkylation. N-(ω-Chloroalkyl) analogs were prepared and subjected to iodide catalyzed nucleophilic substitution reaction with secondary amines to give N-(ω-aminoalkyl) derivs., which enhanced the uptake of vinblastine in KBChR-8-5 cells to a greater extent (2.6-13.1-fold relative to control) than verapamil. The study on the structure-activity relationship revealed that the OMe group at position 4 increased the cytotoxic and anti-MDR activities. The ability of acridones to inhibit calmodulin dependent cAMP phosphodiesterase has been determined and the results have shown a strong pos. correlation between anti-calmodulin activity and cytotoxicity in KBChR-8-5 cells or anti-MDR activity.

RX(57) OF 98 - 3 STEPS

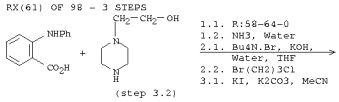


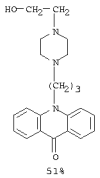
58%

CON: STEP(1.1) 3 hours, 100 deg C
STEP(1.2) >room temperature - <
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 24 hours, room temperature
STEP(3.1) 30 minutes, reflux
STEP(3.2) 15 hours, reflux

L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(61) OF 98 - 3 STEPS

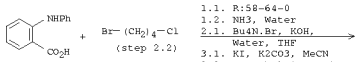


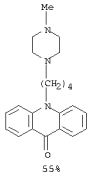


51%

CON: STEP(1.1) 3 hours, 100 deg C
STEP(1.2) >room temperature - <
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 24 hours, room temperature
STEP(3.1) 30 minutes, reflux
STEP(3.2) 15 hours, reflux

RX(62) OF 98 - 3 STEPS



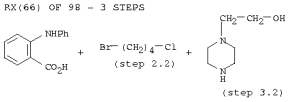


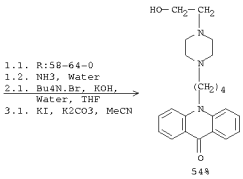
55%

L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

CON: STEP(1.1) 3 hours, 100 deg C
STEP(1.2) >room temperature - <
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 24 hours, room temperature
STEP(3.1) 30 minutes, reflux
STEP(3.2) 15 hours, reflux

RX(66) OF 98 - 3 STEPS

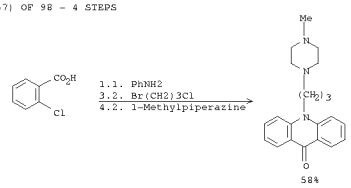




54%

CON: STEP(1.1) 3 hours, 100 deg C
STEP(1.2) >room temperature - <
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 24 hours, room temperature
STEP(3.1) 30 minutes, reflux
STEP(3.2) 15 hours, reflux

RX(67) OF 98 - 4 STEPS

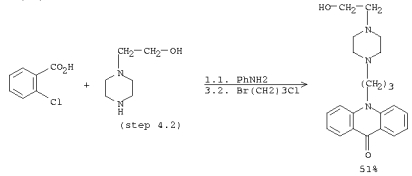


58%

L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

NOTE: 1) Ullmann condensation, activated charcoal used in third stage
CON: STEP(1.1) 6 hours, reflux
STEP(1.2) >room temperature
STEP(1.3) reflux
STEP(2.1) 3 hours, 100 deg C
STEP(2.2) >room temperature - <
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 24 hours, room temperature
STEP(4.1) 30 minutes, reflux
STEP(4.2) 15 hours, reflux

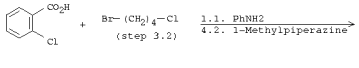
RX(71) OF 98 - 4 STEPS

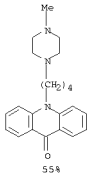


51%

NOTE: 1) Ullmann condensation, activated charcoal used in third stage
CON: STEP(1.1) 6 hours, reflux
STEP(1.2) >room temperature
STEP(1.3) reflux
STEP(2.1) 3 hours, 100 deg C
STEP(2.2) >room temperature - <
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 24 hours, room temperature
STEP(4.1) 30 minutes, reflux
STEP(4.2) 15 hours, reflux

RX(72) OF 98 - 4 STEPS



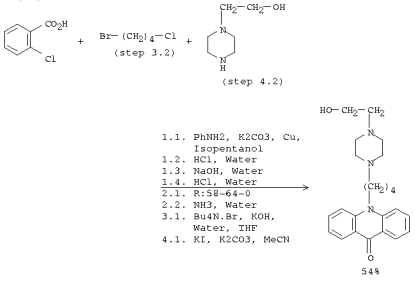


55%

L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

NOTE: 1) Ullmann condensation, activated charcoal used in third stage
CON: STEP(1.1) 6 hours, reflux
STEP(1.2) >room temperature
STEP(1.3) reflux
STEP(2.1) 3 hours, 100 deg C
STEP(2.2) >room temperature - <
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 24 hours, room temperature
STEP(4.1) 30 minutes, reflux
STEP(4.2) 15 hours, reflux

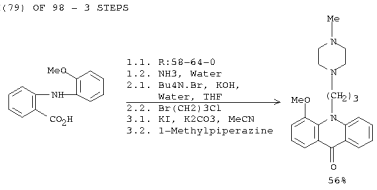
RX(76) OF 98 - 4 STEPS



NOTE: 1) Ullmann condensation, activated charcoal used in third stage
CON: STEP(1.1) 6 hours, reflux
STEP(1.2) >room temperature
STEP(1.3) reflux
STEP(2.1) 3 hours, 100 deg C
STEP(2.2) >room temperature - <
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 24 hours, room temperature
STEP(4.1) 30 minutes, reflux
STEP(4.2) 15 hours, reflux

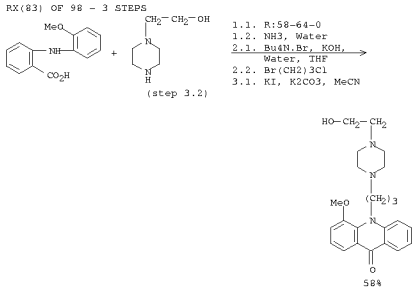
L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(79) OF 98 - 3 STEPS



CON: STEP(1.1) 3 hours, 100 deg C
STEP(1.2) >room temperature - <
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 24 hours, room temperature
STEP(3.1) 30 minutes, reflux
STEP(3.2) 15 hours, reflux

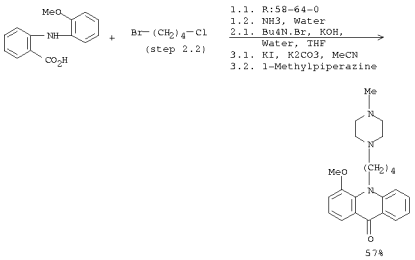
RX(83) OF 98 - 3 STEPS



CON: STEP(1.1) 3 hours, 100 deg C
STEP(1.2) >room temperature - <
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 24 hours, room temperature
STEP(3.1) 30 minutes, reflux
STEP(3.2) 15 hours, reflux

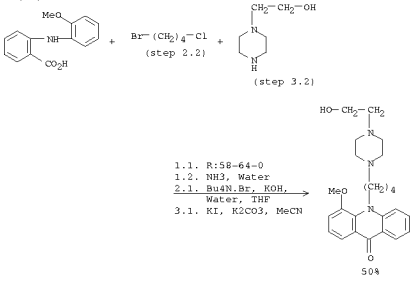
L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(84) OF 98 - 3 STEPS



CON: STEP(1.1) 3 hours, 100 deg C
STEP(1.2) >room temperature - <
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 24 hours, room temperature
STEP(3.1) 30 minutes, reflux
STEP(3.2) 15 hours, reflux

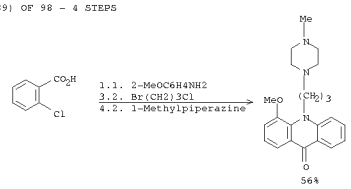
RX(88) OF 98 - 3 STEPS



L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

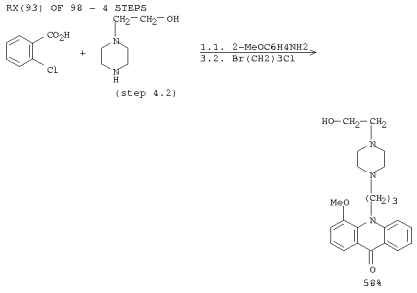
CON: STEP(1.1) 3 hours, 100 deg C
STEP(1.2) >room temperature - <
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 24 hours, room temperature
STEP(3.1) 30 minutes, reflux
STEP(3.2) 15 hours, reflux

RX(89) OF 98 - 4 STEPS



NOTE: 1) Ullmann condensation, activated charcoal used in third stage
CON: STEP(1.1) 6 hours, reflux
STEP(1.2) >room temperature
STEP(1.3) reflux
STEP(2.1) 3 hours, 100 deg C
STEP(2.2) >room temperature - <
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 24 hours, room temperature
STEP(4.1) 30 minutes, reflux
STEP(4.2) 15 hours, reflux

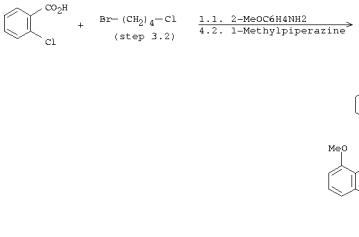
RX(93) OF 98 - 4 STEPS



L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

NOTE: 1) Ullmann condensation, activated charcoal used in third stage
CON: STEP(1.1) 6 hours, reflux
STEP(1.2) >room temperature
STEP(1.3) reflux
STEP(2.1) 3 hours, 100 deg C
STEP(2.2) >room temperature - <
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 24 hours, room temperature
STEP(4.1) 30 minutes, reflux
STEP(4.2) 15 hours, reflux

RX(94) OF 98 - 4 STEPS



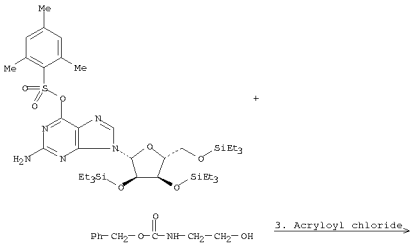
NOTE: 1) Ullmann condensation, activated charcoal used in third stage
CON: STEP(1.1) 6 hours, reflux
STEP(1.2) >room temperature
STEP(1.3) reflux
STEP(2.1) 3 hours, 100 deg C
STEP(2.2) >room temperature - <
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 24 hours, room temperature
STEP(4.1) 30 minutes, reflux
STEP(4.2) 15 hours, reflux

L26 ANSWER 2 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 140:283384 CASREACT
TI Modulators of GTPases and modulator-resistant enzymes and their uses in drug design and target validation
IN Shah, Kavita; Vincent, Fabien; Cuento, Maria A.
PA Irm, Llc, UK; Novartis Pharmaceuticals Corporation
SO PCT Int. Appl., 144 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO--2004024082	A2	20040325	2003WO-US028594	20030910
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU--2003267145	A1	20040430	2003AU-000267145	20030910
US-20040241706	A1	20041202	2003US-000660113	20030910
PRAI 2002US-00410536P		20020913		
2003US-00461755P		20030409		
2003WO-US028594		20030910		

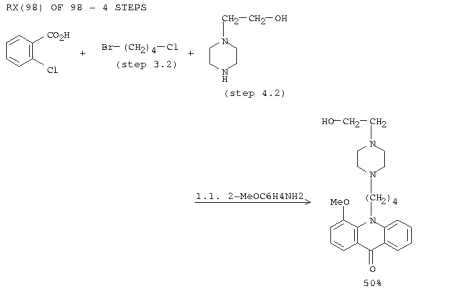
OS MARPAT 140:283384
AB Guanine derivs. that act as modulators of GTPases and GTPase variants that do not interact with these modulators are described for use in the design of improved modulators of GTPase activity. The method involves generating variants of the enzyme that do not interact with a known modulator and then developing effectors that interact with the resistant variant. The preparation of guanosine derivs. and of a series of p21c-Ha-ras protein substitution variants is described,.

RX(461) OF 527 - 6 STEPS



L26 ANSWER 1 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(98) OF 98 - 4 STEPS

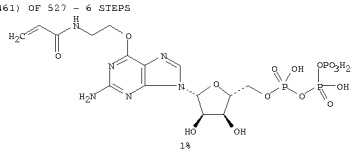


NOTE: 1) Ullmann condensation, activated charcoal used in third stage
CON: STEP(1.1) 6 hours, reflux
STEP(1.2) >room temperature
STEP(1.3) reflux
STEP(2.1) 3 hours, 100 deg C
STEP(2.2) >room temperature - <
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 24 hours, room temperature
STEP(4.1) 30 minutes, reflux
STEP(4.2) 15 hours, reflux

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

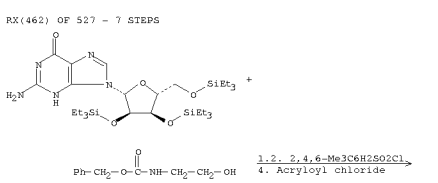
RX(461) OF 527 - 6 STEPS



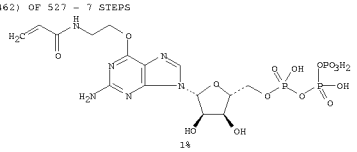
1%

NOTE: 1) molecular sieve used in stage 1, 3) incremental addition of the reactant, 6) Other analogs similarly prepared
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 18 hours, room temperature
STEP(2) 18 hours, room temperature
STEP(3.1) room temperature -> 0 deg C; 1 hour, 0 deg C; 0 deg C -> room temperature; 15 minutes, room temperature
STEP(4) 36 hours, room temperature
STEP(5.1) room temperature -> 4 deg C; 4 deg C; 2 hours, 4 deg C
STEP(5.2) cooled
STEP(6.1) room temperature -> 4 deg C; 2 hours, 4 deg C
STEP(6.2) room temperature; 1 minute, room temperature
STEP(6.3) cooled

RX(462) OF 527 - 7 STEPS



RX(462) OF 527 - 7 STEPS

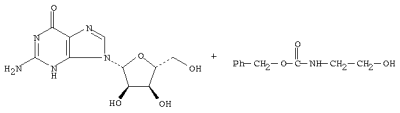


1%

L26 ANSWER 2 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

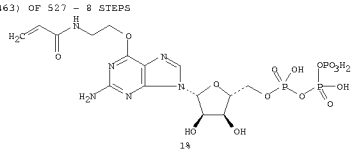
NOTE: 2) molecular sieve used in stage 1, 4) incremental addition of the reactant, 7) Other analogs similarly prepared
CON: STEP(1.1) 15 minutes, room temperature -> 0 deg C
STEP(1.2) 4 hours, 0 deg C; 18 hours, 0 deg C -> room temperature
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 18 hours, room temperature
STEP(3) 18 hours, room temperature
STEP(4.1) room temperature -> 0 deg C; 1 hour, 0 deg C; 0 deg C -> room temperature; 15 minutes, room temperature
STEP(5) 36 hours, room temperature
STEP(6.1) room temperature -> 4 deg C; 4 deg C; 2 hours, 4 deg C
STEP(6.2) cooled
STEP(7.1) room temperature -> 4 deg C; 2 hours, 4 deg C
STEP(7.2) room temperature; 1 minute, room temperature
STEP(7.3) cooled

RX(463) OF 527 - 8 STEPS



1. Et3SiCl
2.2. 2,4,6-Me3C6H2SO2Cl
5. Acryloyl chloride

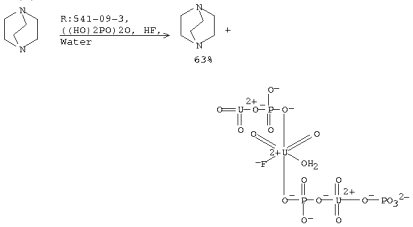
RX(463) OF 527 - 8 STEPS



1%

L26 ANSWER 3 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 140:280230 CASREACT
TI [N2C6H14]2[(UO2)6(H2O)2F2(PO4)2(HPO4)4]·4H2O: A New Microporous Uranium Phosphate Fluoride
AU Doran, Michael B.; Stuart, Clair L.; Norquist, Alexander J.; O'Hare, Dermot
CS Inorganic Chemistry Laboratory, University of Oxford, Oxford, OX1 3QR, UK
SO Chemistry of Materials (2004), 16(4), 565-566
CODEN: CMATEX; ISSN: 0897-4756
PB American Chemical Society
DT Journal
LA English
AB The phase-pure preparation, crystal structure and thermal stability of microporous [N2C6H14]2[(UO2)6(H2O)2F2(PO4)2(HPO4)4]·4H2O (MUPF-1) (I) are reported. I was prepared from UO2(NO3)2, H4P2O7 and HF in aqueous solution in presence of DABCO. I is monoclinic, space group P21/n, Z = 4, R = 0.0399, Rw = 0.0988. I decomposed to U2O(PO)4 at 800° with decomposition beginning at 40°.

RX(1) OF 1



R:541-09-3,
((HO)2PO)2O, HF,
Water

63%

4 H+
63%

NOTE: autoclave used, hydrothermal conditions
CON: STAGE(1) 24 hours, 180 deg C; 180 deg C -> room temperature

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

NOTE: 1) incremental addition of the reactant, 3) molecular sieve used in stage 1, 5) incremental addition of the reactant, 8) Other analogs similarly prepared
CON: STEP(1.1) room temperature -> 0 deg C; 30 minutes, 0 deg C; 3 hours, 0 deg C -> room temperature
STEP(2.1) 15 minutes, room temperature -> 0 deg C
STEP(2.2) 4 hours, 0 deg C; 18 hours, 0 deg C -> room temperature
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 18 hours, room temperature
STEP(4) 18 hours, room temperature
STEP(5.1) room temperature -> 0 deg C; 1 hour, 0 deg C; 0 deg C -> room temperature; 15 minutes, room temperature
STEP(6) 36 hours, room temperature
STEP(7.1) room temperature -> 4 deg C; 4 deg C; 2 hours, 4 deg C
STEP(7.2) cooled
STEP(8.1) room temperature -> 4 deg C; 2 hours, 4 deg C
STEP(8.2) room temperature; 1 minute, room temperature
STEP(8.3) cooled

L26 ANSWER 4 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 140:111626 CASREACT
TI Chemoenzymatic Synthesis and Antibody Detection of DNA Glycoconjugates
AU Wang, Yingli; Sheppard, Terry L.
CS Department of Chemistry and The Robert H. Lurie Comprehensive Cancer Center, Northwestern University, Evanston, IL, 60208-3113, USA
SO Bioconjugate Chemistry (2003), 14(6), 1314-1322
CODEN: BCCHES; ISSN: 1043-1802
PB American Chemical Society
DT Journal
LA English
AB A chemoenzymic approach for the efficient synthesis of DNA-carbohydrate conjugates was developed and applied to an antibody-based strategy for the detection of DNA glycoconjugates. A phosphoramidite derivative of N-acetylglucosamine (GlcNAc) was synthesized and utilized to attach GlcNAc sugars to the 5'-terminus of DNA oligonucleotides by solid-phase DNA synthesis. The resulting GlcNAc-DNA conjugates were used as substrates for glycosyl transferase enzymes to synthesize DNA glycoconjugates. Treatment of GlcNAc-DNA with β-1,4-galactosyl transferase (GalT) and UDP-Gal produced N-acetyllactosamine-modified DNA (LacNAc-DNA), which could be converted quant. to the trisaccharide Lewis X (LeX)-DNA conjugate by α-1,3-fucosyltransferase VI (FucT) and GDP-Fuc. The facile enzymic synthesis of LeX-DNA from GlcNAc-DNA also was accomplished in a one-pot reaction by the combined action of GalT and FucT. The resulting glycoconjugates were characterized by gel electrophoresis, matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF MS), and glycosidase digestion expts. Covalent modification of the 5'-terminus of DNA with carbohydrates did not interfere with the ability of DNA glycoconjugates to hybridize with complementary DNA, as indicated by UV thermal denaturation anal. The trisaccharide DNA glycoconjugate, LeX-DNA, was detected by a dual DNA hybridization/monoclonal antibody (mAb) detection protocol ("Southwestern"): membrane-immobilized LeX-DNA was visualized by Southern detection with a radiolabeled complementary DNA probe and by Western chemiluminescence detection with a mAb specific for the LeX antigen. The efficient chemoenzymic synthesis of DNA glycoconjugates and the Southwestern detection protocol may facilitate the application of glycosylated DNA to cellular targeting and DNA glycoconjugate detection strategies.

RX(6) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(7) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(8) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(9) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(13) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(14) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(16) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(17) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(19) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(20) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(21) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(22) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(23) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(24) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(25) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(26) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(31) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(32) OF 34 - REACTION DIAGRAM NOT AVAILABLE

L26 ANSWER 4 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)
RX(33) OF 34 - REACTION DIAGRAM NOT AVAILABLE

RX(34) OF 34 - REACTION DIAGRAM NOT AVAILABLE
RE.CNT 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 5 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 140:59885 CASREACT
TI First enzymatic synthesis of an N1-cyclized cADPR (cyclic-ADP ribose) analogue with a hypoxanthine partial structure: discovery of a membrane permeant cADPR agonist
AU Wagner, Gerd K.; Black, Steven; Guse, Andreas H.; Potter, Barry V. L.
CS Department of Pharmacy and Pharmacology, Wolfson Laboratory of Medicinal Chemistry, University of Bath, Bath, BA2 7AY, UK
SO Chemical Communications (Cambridge, United Kingdom) (2003), (15), 1944-1945
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
AB Nicotinamide 8-Br-hypoxanthine dinucleotide (8-Br-NHD+) was cyclized at the N1 position by the ADP-ribosyl cyclase from Aplysia californica to give cyclic 8-Br-inosine diphosphoribose (8-Br-N1-cIDPR), a novel membrane-permeant agonist of Ca2+ release in human T cells.

RX(1) OF 1 - REACTION DIAGRAM NOT AVAILABLE
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 6 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 139:261490 CASREACT
TI An efficient synthesis of a biantennary sialooligosaccharide analog using a 1,6-anhydro-β-lactose derivative as a key synthetic block
AU Furuike, Tetsuya; Yamada, Kuriko; Ohta, Takashi; Monde, Kenji; Nishimura, Shin-Ichiro
CS Japan Bioindustry Association, Sapporo Laboratory for Glycocluster Project, Hokkaido University, Sapporo, 060-0810, Japan
SO Tetrahedron (2003), 59(27), 5105-5113
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science B.V.
DT Journal
LA English
AB An efficient and versatile method for the synthesis of a biantennary octasaccharide derivative was established by combined chemical and enzymic manipulations of 1,6-anhydro-β-lactose as a key starting material. A key 1,6-anhydro-β-lactose derivative having two unprotected hydroxyl groups at C-3' and C-6' positions was prepared and employed for the chemical coupling reaction with a known 3,4,6-tri-O-acetyl-2-deoxy-2-phthalimido-β-D-glucopyranosyl imidate to afford a tetrasaccharide derivative with two GlcNAc branches in 69% yield. Enzymic galactosylation using UDP-Gal with a bovine milk β1,4-galactosyltransferase and subsequent sialylation with a recombinant α2,3-sialyltransferase in the presence of CMP-Neu5Ac proceeded smoothly and gave a desired model compound, a bivalent sialooctasaccharide, in 73% overall yield from the tetrasaccharide intermediate.

RX(13) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(26) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(27) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(47) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(48) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(49) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(50) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(77) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(78) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(79) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(80) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(81) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(82) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(83) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(84) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(95) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(96) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(97) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(98) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(99) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(100) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(101) OF 105 - REACTION DIAGRAM NOT AVAILABLE

RX(102) OF 105 - REACTION DIAGRAM NOT AVAILABLE

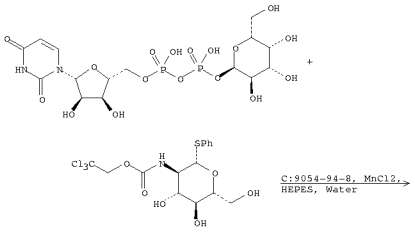
RX(103) OF 105 - REACTION DIAGRAM NOT AVAILABLE

L26 ANSWER 6 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)
RX(104) OF 105 - REACTION DIAGRAM NOT AVAILABLE

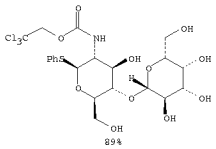
RX(105) OF 105 - REACTION DIAGRAM NOT AVAILABLE
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 7 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 138:338378 CASREACT
TI Simplifying Oligosaccharide Synthesis: Efficient Synthesis of Lactosamine and Sialylated Lactosamine Oligosaccharide Donors
AU Yan, Fengyang; Mehta, Seema; Eichler, Eva; Wakarchuk, Warren W.; Gilbert, Michel; Schur, Melissa J.; Whitfield, Dennis M.
CS Institute for Biological Sciences, National Research Council of Canada, Ottawa, ON, K1A 0R6, Can.
SO Journal of Organic Chemistry (2003), 68(6), 2426-2431
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB A practical sequence is described for converting D-glucosamine into peracetylated Gal(β-1,4)GlcNTroc(β1-S)Ph and Neu5Ac(α-2,3)Gal(β-1,4)GlcNTroc(β1-S)Ph building blocks using a synthetic strategy based on chemoenzymic oligosaccharide synthesis. The known trichloroethoxycarbonyl, N-Troc, protecting group was selected as a suitable protecting group for both enzymic and chemical reaction conditions. These oligosaccharide building blocks proved effective donors for the β-selective glycosylation of the un-reactive OH-3 of a polymeric PEG-bound acceptor and for the axial OH-2 of a mannose acceptor in good yields. The resulting complex oligosaccharides are useful for vaccine and pharmaceutical applications.

RX(3) OF 45



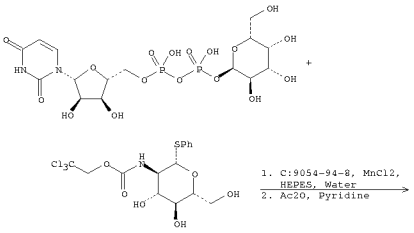
RX(3) OF 45



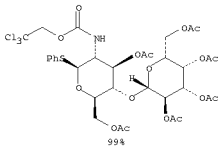
NOTE: biotransformation, enzymic, stereoselective, buffered soln.
CON: 20 hours, 37 deg C, pH 7.4

L26 ANSWER 7 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(16) OF 45 - 2 STEPS

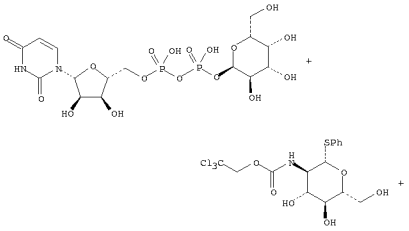


RX(16) OF 45 - 2 STEPS



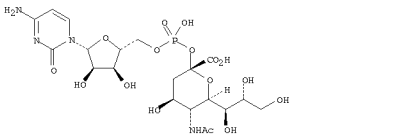
NOTE: 1) biotransformation, enzymic, stereoselective, buffered soln.
CON: STEP(1) 20 hours, 37 deg C, pH 7.4
STEP(2.1) 0 deg C; 16 hours, room temperature

RX(17) OF 45 - 2 STEPS

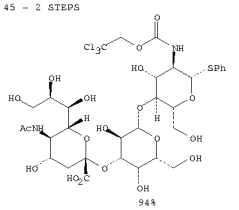


L26 ANSWER 7 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(17) OF 45 - 2 STEPS



RX(17) OF 45 - 2 STEPS

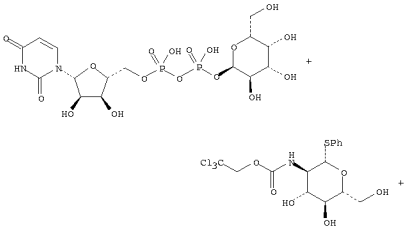


NOTE: 1) biotransformation, enzymic, stereoselective, buffered soln.,
2) biotransformation, enzymic, stereoselective, buffered soln.
CON: STEP(1) 20 hours, 37 deg C, pH 7.4
STEP(2.1) 37 deg C
STEP(2.2) 2 hours, 37 deg C

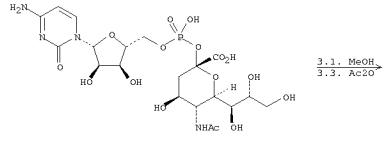
RX(27) OF 45 - REACTION DIAGRAM NOT AVAILABLE

L26 ANSWER 7 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

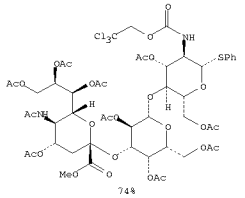
RX(28) OF 45 - 3 STEPS



RX(28) OF 45 - 3 STEPS



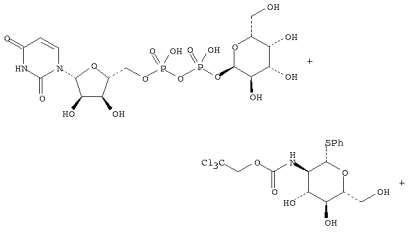
RX(28) OF 45 - 3 STEPS



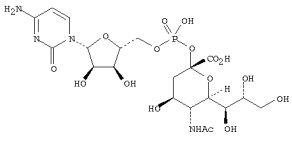
NOTE: 1) biotransformation, enzymic, stereoselective, buffered soln.,
2) biotransformation, enzymic, stereoselective, buffered soln.,
3) other product also detected, Dowex 500WX8-200 (H+) used
CON: STEP(1) 20 hours, 37 deg C, pH 7.4
STEP(2.1) 37 deg C
STEP(2.2) 2 hours, 37 deg C
STEP(3.1) 16 hours, room temperature
STEP(3.3) 2 hours, room temperature

L26 ANSWER 7 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(29) OF 45 - 3 STEPS



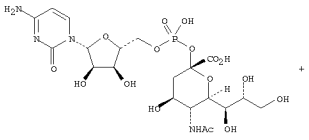
RX(29) OF 45 - 3 STEPS

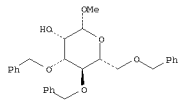


1. C:9054-94-8, MnCl2, HEPES, Water
2.1. MgCl2, R:4432-31-9, Water
2.2. C:71124-51-1
3.1. Ac2O, Pyridine
3.2. PhMe

L26 ANSWER 7 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

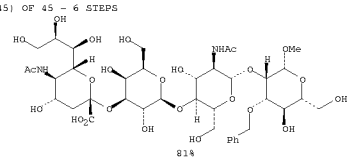
RX(45) OF 45 - 6 STEPS





3.1. MeOH
3.3. Ac2O
5.1. Ac2O
6.5. MeOH

RX(45) OF 45 - 6 STEPS



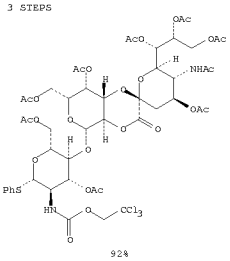
81%

NOTE: 1) biotransformation, enzymic, stereoselective, buffered soln., 2) biotransformation, enzymic, stereoselective, buffered soln., 3) other product also detected, Dowex 500wx8-200 (H+) used, 4) stereoselective, 6) rexyn 101 (H+) used
CON: STEP(1) 20 hours, 37 deg C, pH 7.4
STEP(2.1) 37 deg C
STEP(2.2) 2 hours, 37 deg C
STEP(3.1) 16 hours, room temperature
STEP(3.3) 2 hours, room temperature
STEP(4) 2 hours, room temperature
STEP(5) overnight, room temperature
STEP(6.1) 16 hours, room temperature, 50 psi
STEP(6.2) 2 hours, room temperature
STEP(6.3) neutralized
STEP(6.4) overnight, room temperature
STEP(6.6) neutralized

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 7 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(29) OF 45 - 3 STEPS



92%

NOTE: 1) biotransformation, enzymic, stereoselective, buffered soln., 2) biotransformation, enzymic, stereoselective, buffered soln.
CON: STEP(1) 20 hours, 37 deg C, pH 7.4
STEP(2.1) 37 deg C
STEP(2.2) 2 hours, 37 deg C
STEP(3.1) 0 deg C; 18 hours, 45 deg C

RX(35) OF 45 - REACTION DIAGRAM NOT AVAILABLE

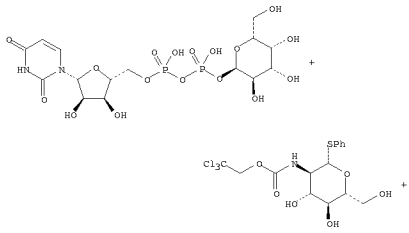
RX(37) OF 45 - REACTION DIAGRAM NOT AVAILABLE

RX(40) OF 45 - REACTION DIAGRAM NOT AVAILABLE

RX(41) OF 45 - REACTION DIAGRAM NOT AVAILABLE

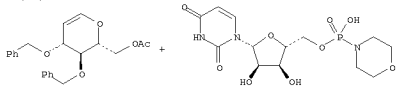
RX(42) OF 45 - REACTION DIAGRAM NOT AVAILABLE

RX(45) OF 45 - 6 STEPS



L26 ANSWER 8 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 138:73454 CASREACT
TI A direct synthesis of 2-deoxy-2-fluoro-α-D-[6-3H]glucopyranosyl uridine-5'-diphosphate
AU Stick, Robert V.; Watts, Andrew G.
CS Department of Chemistry, The University of Western Australia, Crawley, 6009, Australia
SO Australian Journal of Chemistry (2002), 55(5), 327-329
CODEN: AJCHAS; ISSN: 0004-9425
PB CSIRO Publishing
DT Journal
LA English
AB The synthesis of 2-deoxy-2-fluoro-α-D-[6-3H]glucopyranosyl uridine-5'-diphosphate, with the late introduction of the radiolabel, has been achieved from 3,4-di-O-benzyl-2-deoxy-2-fluoro-α-D-glucosyl di-Ph phosphate, by an oxidation-reduction sequence, followed by protecting group removal and morpholidate coupling to uridine-5'-monophosphate.

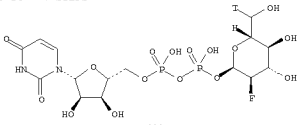
RX(35) OF 36 - 7 STEPS



(step 7)

2.1. (PhO)2P(O)Cl
6.3. Bu3N
7. Carboxamidine deriv.

RX(35) OF 36 - 7 STEPS

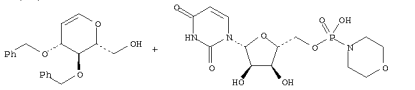


68%

NOTE: 1) stereoselective, 2) stereoselective, 3) stereoselective, Amberlite IR-120(H+) used, 4) stereoselective, mol. sieves used, 5) stereoselective, 6) Dowex 50w-x8 (H+) used, 7) literature prepn.
CON: STEP(1) 3 hours, room temperature
STEP(2.1) -10 deg C; 1 hour, -10 deg C
STEP(3) 40 hours, 0 deg C
STEP(4) 1 hour, room temperature
STEP(5.1) 30 minutes, room temperature
STEP(5.2) 30 minutes, room temperature
STEP(5.3) room temperature
STEP(6.1) 2 hours, room temperature
STEP(6.2) overnight, room temperature

L26 ANSWER 8 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

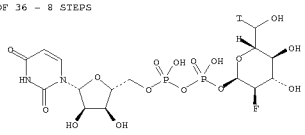
RX(36) OF 36 - 8 STEPS



(step 8)

1.1. AcCl
3.1. (PhO)2P(O)Cl
7.3. Bu3N
8. Carboxamidine deriv.

RX(36) OF 36 - 8 STEPS



68%

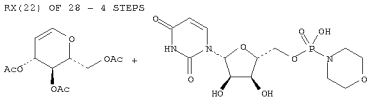
NOTE: 1) stereoselective, 2) stereoselective, 3) stereoselective, 4) stereoselective, Amberlite IR-120(H+) used, 5) stereoselective, mol. sieves used, 6) stereoselective, 7) Dowex 50w-x8 (H+) used, 8) literature prepn.
CON: STEP(1) 1 hour, room temperature
STEP(2) 3 hours, room temperature
STEP(3.1) -10 deg C; 1 hour, -10 deg C
STEP(4) 40 hours, 0 deg C
STEP(5) 1 hour, room temperature
STEP(6.1) 30 minutes, room temperature
STEP(6.2) 30 minutes, room temperature
STEP(6.3) room temperature
STEP(7.1) 2 hours, room temperature
STEP(7.2) overnight, room temperature

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 9 OF 25 CASREACT COPYRIGHT 2008 ACS on STN

AN 137:201516 CASREACT
TI The chameleon of retaining glycoside hydrolases and retaining glycosyl transferases: the catalytic nucleophile
AU Stick, Robert V.; Watts, Andrew G.
CS Department of Chemistry, The University of Western Australia, Crawley, 6009, Australia
SO Monatshefte fuer Chemie (2002), 133(4), 541-554
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer-Verlag Wien
DT Journal; General Review
LA English
AB The authors report reliable procedures for the synthesis of various 2-deoxy-2-fluoro glycosyl nucleoside diphosphates, useful donor analogs for the study of the mechanism of action of retaining glycosyltransferases. The existence and role of a catalytic nucleophile in retaining glycoside hydrolases and retaining glycosyltransferases are reviewed. Although the former has now been established beyond doubt, such is not the case with the latter.

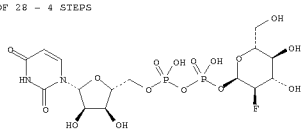
RX(22) OF 28 - 4 STEPS



(step 4.3)

1.2. Ac2O
2.2. AcOH
3.3. Dicyclohexylamine
4.3. Carboxamidine deriv.

RX(22) OF 28 - 4 STEPS

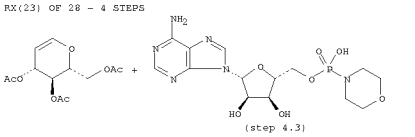


68%

NOTE: 1) stereoselective, 2) stereoselective, 3) MacDonald phosphorylation, stereoselective, 4) Dowex 50W-X8 in H+ form used after step 1

L26 ANSWER 9 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

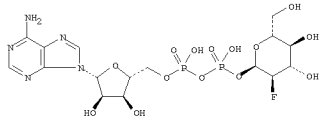
RX(23) OF 28 - 4 STEPS



(step 4.3)

1.2. Ac2O
2.2. AcOH
3.3. Dicyclohexylamine
4.3. Carboxamidine deriv.

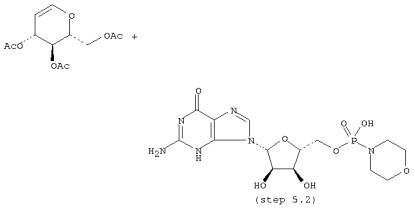
RX(23) OF 28 - 4 STEPS



71%

NOTE: 1) stereoselective, 2) stereoselective, 3) MacDonald phosphorylation, stereoselective, 4) Dowex 50W-X8 in H+ form used after step 1

RX(28) OF 28 - 5 STEPS

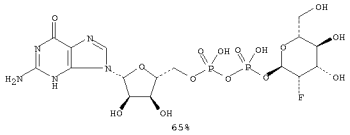


(step 5.2)

L26 ANSWER 9 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(28) OF 28 - 5 STEPS

1.2. Ac2O
3.2. (PhO)2P(O)Cl
4.3. Bu3N
5.2. Carboxamidine deriv.



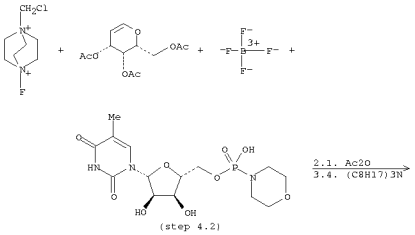
65%

NOTE: 1) stereoselective, 4) Dowex 50W-X8 in H+ form used after step 2

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

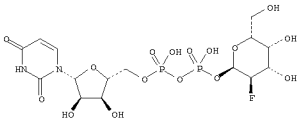
L26 ANSWER 10 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 137:2344 CASREACT
TI Mechanistic Studies of a Retaining α-Galactosyltransferase from Neisseria meningitidis
AU Ly, Hoa D.; Lougheed, Brenda; Wakarchuk, Warren W.; Withers, Stephen G.
CS Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SO Biochemistry (2002), 41(16), 5075-5085
CODEN: BICHAW; ISSN: 0006-2960
PB American Chemical Society
DT Journal
LA English
AB Lipopolysaccharyl α-galactosyltransferase from Neisseria meningitidis catalyzes the transfer of a galactosyl moiety from the activated donor UDP-Gal to glycoconjugates to yield an elongated saccharide product with net retention of anomeric configuration relative to the donor substrate. Through kinetic analyses in which the concns. of both substrates are independently varied and through inhibition studies with dead-end analogs of both substrates and with the oligosaccharide product, we have demonstrated that this enzyme follows an ordered bi-bi kinetic mechanism. Various aspects of the chemical mechanism including the possible formation of a covalent glycosyl-enzyme intermediate were also probed using an assortment of strategies. While the results of these investigations were unable to clearly delineate the chemical mechanism of this enzyme, they provide important insights into the catalytic machinery surrounding the events involved in catalysis.

RX(69) OF 118 - 4 STEPS



L26 ANSWER 10 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(69) OF 118 - 4 STEPS

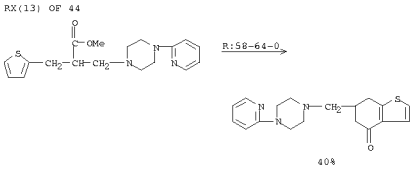


NOTE: 1) stereoselective, 2) stereoselective, 3) sulfonic acid exchanger used, stereoselective, 4) stereoselective

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

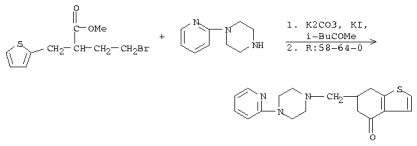
L26 ANSWER 11 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 136:160857 CASREACT
TI New Serotonin 5-HT2A, 5-HT2B, and 5-HT2C Receptor Antagonists: Synthesis, Pharmacology, 3D-QSAR, and Molecular Modeling of (Aminoalkyl)benzo and Heterocycloalkanones
AU Brea, Jose; Rodrigo, Jordi; Carrieri, Antonio; Sanz, Ferran; Cadavid, M. Isabel; Enguix, Maria J.; Villazon, Maria; Mengod, Guadalupe; Caro, Yolanda; Masaguer, Christian F.; Ravina, Enrique; Centeno, Nuria B.; Carotti, Angelo; Loza, M. Isabel
CS Departamento de Farmacologia Facultad de Farmacia, Universidad de Santiago de Compostela, Santiago de Compostela, E-15782, Spain
SO Journal of Medicinal Chemistry (2002), 45(1), 54-71
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB A series of 52 conformationally constrained butyrophenones have been synthesized and pharmacol. tested as antagonists at 5-HT2A, 5-HT2B, and 5-HT2C serotonin receptors, useful for dissecting the role of each 5-HT2 subtype in pathophysiol. These compds. were also a consistent set for the identification of structural features relevant to receptor recognition and subtype discrimination. Six compds. were found highly active (pKi > 8.76) and selective at the 5-HT2A receptor vs. 5-HT2B and/or 5-HT2C receptors. Piperidine fragments confer high affinity at the 5-HT2A receptor subtype, with benzofuranone- and thiotetralonepiperidine as the most selective derivs. over 5-HT2C and 5-HT2B receptors, resp.; Ki 2A/2C and/or KB 2A/2B ratios greater than 100 were obtained. Compds. showing a more pronounced selectivity at 5-HT2A/5-HT2C than at 5-HT2A/5-HT2B bear 6-fluorobenzisoxazolyl- and p-fluorobenzoylpiperidine moieties containing one methylene bridging the basic piperidine to the alkanone moiety. An ethylene bridge between the alkanone and the amino moieties led to ligands with higher affinities for the 5-HT2B receptor. Significant selectivity at the 5-HT2B receptor vs. 5-HT2C was observed with 1-1[(1-oxo-1,2,3,4-tetrahydro-3-naphthyl)methyl]-4-[3-(p-fluorobenzoyl)propyl]piperazine (more than 100-fold higher). Although piperidine fragments also confer higher affinity at 5-HT2C receptors, only piperazine-containing ligands were selective over 5-HT2A. Moderate selectivity was observed at 5-HT2C vs. 5-HT2B (10-fold) with some compds. bearing a 4-[3-(6-fluorobenzisoxazolyl]]piperidine moiety in its structure. Mol. determinants for antagonists acting at 5-HT2A receptors were identified by 3D-QSAR (GRID-GOLPE) studies. Docking simulations at 5-HT2A and 5-HT2C receptors suggest a binding site for the studied type of antagonists (between transmembrane helixes 2, 3, and 7) different to that of the natural agonist serotonin (between 3, 5, and 6).

RX(13) OF 44



L26 ANSWER 11 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(23) OF 44 - 2 STEPS



RE.CNT 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 12 OF 25 CASREACT COPYRIGHT 2008 ACS on STN

AN 135:371915 CASREACT

TI Chemoenzymatic Iterative Synthesis of Difficult Linkages of Oligosaccharides on Soluble Polymeric Supports

AU Yan, Fengyang; Gilbert, Michel; Wakarchuk, Warren W.; Brisson, Jean-Robert; Whitfield, Dennis M.

CS Institute for Biological Sciences, National Research Council of Canada, Ottawa, ON, K1A 0R6, Can.

SO Organic Letters (2001), 3(21), 3265-3268
CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

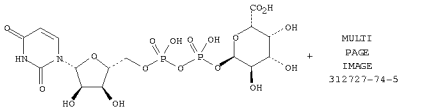
AB A trisaccharide donor containing a cis-Galpα(1→4)Galp linkage was prepared using a synthetic strategy based on chemoenzymic oligosaccharide synthesis on a soluble polymeric support. Significantly, only retaining glycosyltransferases gave complete reactions, whereas inverting enzymes showed little or no activity with poly(ethylene glycol) (MPEG)-bound lactose as an acceptor. The MPEG-attached trisaccharide was shown to bind to Verotoxin-1 by transfer NOE studies through the Galpα(1→4)Galp portion of the mol.

RX(3) OF 25 - REACTION DIAGRAM NOT AVAILABLE

RX(8) OF 25 - REACTION DIAGRAM NOT AVAILABLE

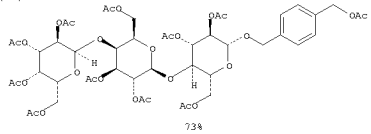
RX(10) OF 25 - REACTION DIAGRAM NOT AVAILABLE

RX(11) OF 25 - 2 STEPS



1. C:212326-70-0, MnCl2, Cleland's reagent, HEPES, Water
2.1. Ac2O, CH2Cl2
2.2. C:144026-79-9

RX(11) OF 25 - 2 STEPS

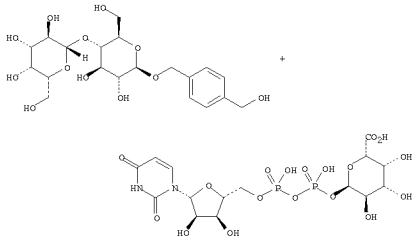


73%

NOTE: 1) no exptl. details, regioselective, buffered soln., biotransformation, enzymic

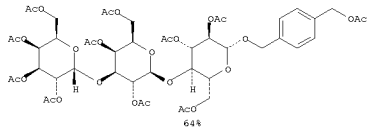
L26 ANSWER 12 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(15) OF 25 - 2 STEPS



RX(15) OF 25 - 2 STEPS

1. C:128449-51-4, MnCl2, HEPES, Water
2.1. Ac2O, CH2Cl2
2.2. C:144026-79-9

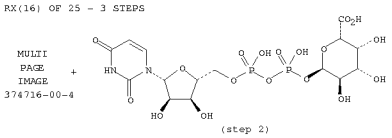


64%

NOTE: 1) no exptl. details, regioselective, buffered soln., biotransformation, enzymic, acetyl bovine serum albumin used

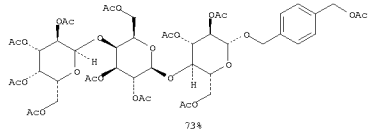
L26 ANSWER 12 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(16) OF 25 - 3 STEPS



1. NaOMe
2. C:212326-70-0, MnCl2, Cleland's reagent, HEPES, Water
3.1. Ac2O, CH2Cl2
3.2. C:144026-79-9

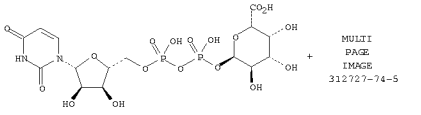
RX(16) OF 25 - 3 STEPS



73%

NOTE: 1) no exptl. details, 2) no exptl. details, regioselective, buffered soln., biotransformation, enzymic

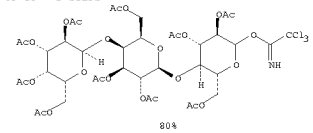
RX(17) OF 25 - 3 STEPS



1. C:212326-70-0, MnCl2, Cleland's reagent, HEPES, Water
2.1. Ac2O, CH2Cl2
2.2. C:144026-79-9
3.1. Pd, H2, MeOH
3.2. Cl3CCN, DBU, CH2Cl2

L26 ANSWER 12 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

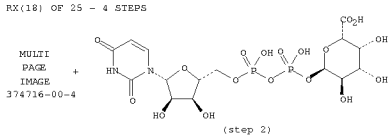
RX(17) OF 25 - 3 STEPS



80%

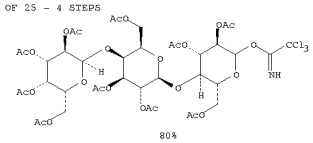
NOTE: 1) no exptl. details, regioselective, buffered soln., biotransformation, enzymic

RX(18) OF 25 - 4 STEPS



1. NaOMe
2. C:212326-70-0, MnCl2, Cleland's reagent, HEPES, Water
3.1. Ac2O, CH2Cl2
3.2. C:144026-79-9
4.1. Pd, H2, MeOH
4.2. Cl3CCN, DBU, CH2Cl2

RX(18) OF 25 - 4 STEPS



80%

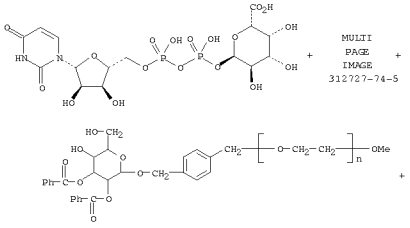
NOTE: 1) no exptl. details, 2) no exptl. details, regioselective, buffered soln., biotransformation, enzymic

RX(20) OF 25 - REACTION DIAGRAM NOT AVAILABLE

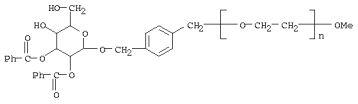
RX(23) OF 25 - REACTION DIAGRAM NOT AVAILABLE

L26 ANSWER 12 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(24) OF 25 - 5 STEPS



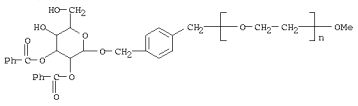
RX(24) OF 25 - 5 STEPS



2.1. Ac2O
3.2. Cl3CCN
5.1. Ac2O

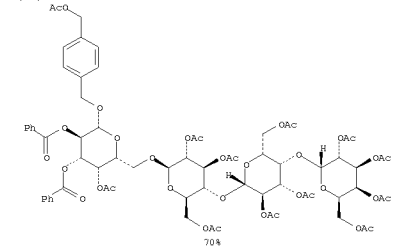
L26 ANSWER 12 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(25) OF 25 - 6 STEPS



3.1. Ac2O
4.2. Cl3CCN
6.1. Ac2O

RX(25) OF 25 - 6 STEPS

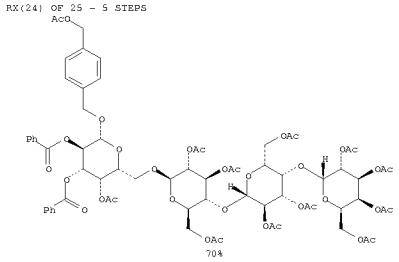


NOTE: 1) no exptl. details, 2) no exptl. details, regioselective, buffered soln., biotransformation, enzymic

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

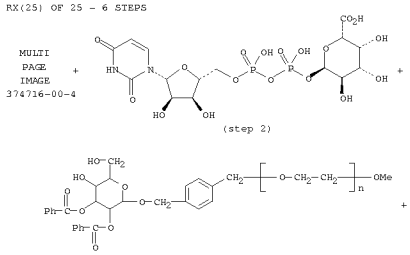
L26 ANSWER 12 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(24) OF 25 - 5 STEPS

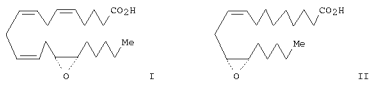


NOTE: 1) no exptl. details, regioselective, buffered soln., biotransformation, enzymic

RX(25) OF 25 - 6 STEPS

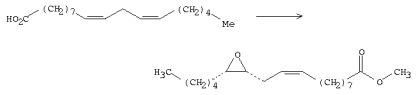


L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 135:226802 CASREACT
TI Practical, enantiospecific syntheses of 14,15-EET and leukotoxin B (vernolic acid)
AU Falck, J. R.; Reddy, Y. K.; Haines, D. C.; Reddy, K. M.; Krishna, U. M.; Graham, S.; Murry, B.; Peterson, J. A.
CS Department of Biochemistry, University of Texas Southwestern Medical Center, Dallas, TX, 75390-9038, USA
SO Tetrahedron Letters (2001), 42(25), 4131-4133
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
GI



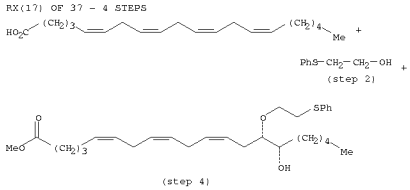
AB Cytochrome P450BM3 and its F87V mutant were exploited for a convenient, laboratory scale (1 mmol) preparation of 14(S),15(R)-epoxyeicosatrienoic acid [14(S),15(R)-EET] (I) from arachidonic acid and (+)-leukotoxin B [(+)-12(S),13(R)-vernolic acid] (II) from linoleic acid, resp. Their enantiomers were accessed via a four-step chemical inversion.

RX(14) OF 37 - 2 STEPS



NOTE: 1) stereoselective, buffered soln., biotransformation, enzymic, 2) stereoselective

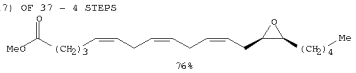
RX(17) OF 37 - 4 STEPS



1.4. CH2N2
3.1. TsCl

L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

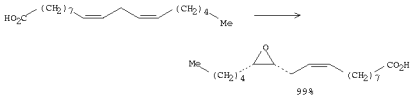
RX(17) OF 37 - 4 STEPS



76%

NOTE: 1) buffered soln., stereoselective, 2) 76% overall yield, stereoselective, 3) 58% overall yield, 4) stereoselective

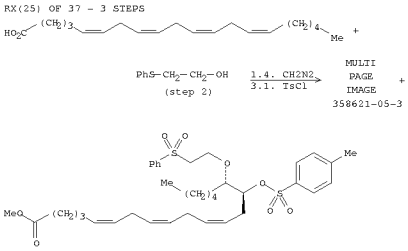
RX(24) OF 37 - 3 STEPS



99%

NOTE: 1) stereoselective, buffered soln., biotransformation, enzymic, 2) stereoselective

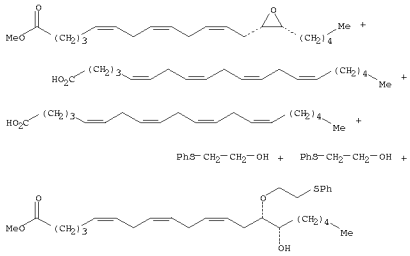
RX(25) OF 37 - 3 STEPS



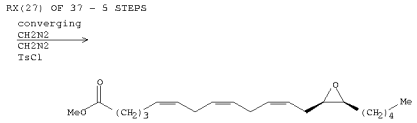
NOTE: 1) buffered soln., stereoselective, 2) 76% overall yield, stereoselective, 3) 58% overall yield

L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(27) OF 37 - 5 STEPS



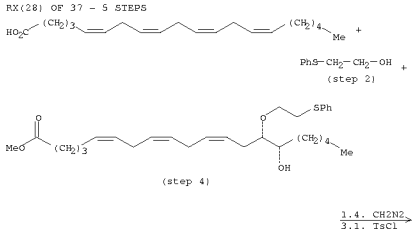
RX(27) OF 37 - 5 STEPS



76%

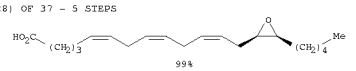
NOTE: buffered soln., stereoselective, 76% overall yield, stereoselective, 58% overall yield, stereoselective, 76% overall yield, stereoselective

RX(28) OF 37 - 5 STEPS



L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

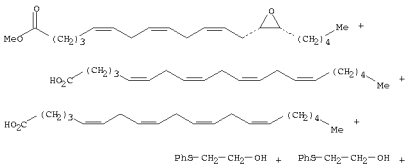
RX(28) OF 37 - 5 STEPS



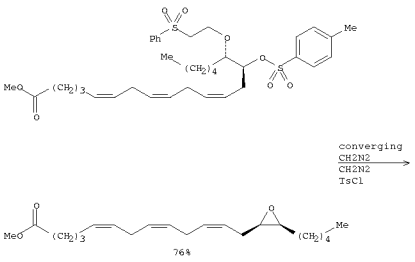
99%

NOTE: 1) buffered soln., stereoselective, 2) 76% overall yield, stereoselective, 3) 58% overall yield, 4) stereoselective

RX(30) OF 37 - 5 STEPS



RX(30) OF 37 - 5 STEPS

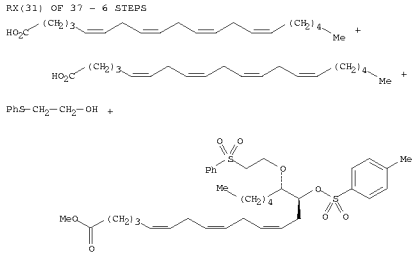


76%

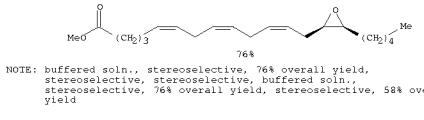
NOTE: buffered soln., stereoselective, 76% overall yield, stereoselective, stereoselective, 76% overall yield, stereoselective, 58% overall yield

L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(31) OF 37 - 6 STEPS



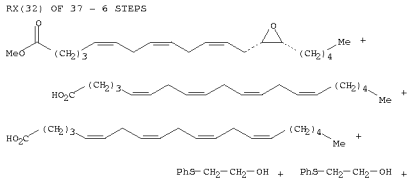
RX(31) OF 37 - 6 STEPS



76%

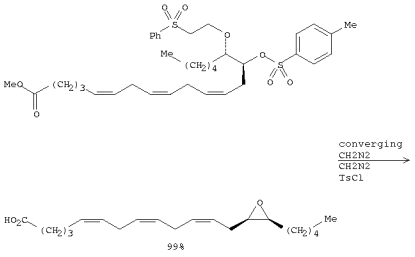
NOTE: buffered soln., stereoselective, 76% overall yield, stereoselective, stereoselective, buffered soln., stereoselective, 76% overall yield, stereoselective, 58% overall yield

RX(32) OF 37 - 6 STEPS



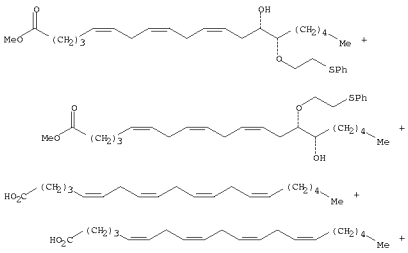
L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(32) OF 37 - 6 STEPS



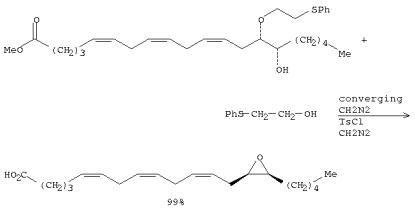
NOTE: buffered soln., stereoselective, 76% overall yield, stereoselective, stereoselective, 76% overall yield, stereoselective, 58% overall yield

RX(34) OF 37 - 5 STEPS



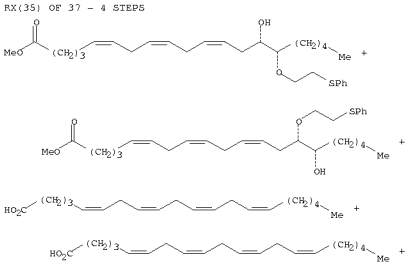
L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(34) OF 37 - 5 STEPS



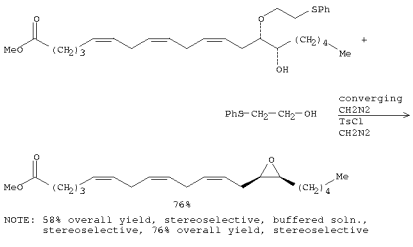
NOTE: 58% overall yield, stereoselective, buffered soln., stereoselective, 76% overall yield, stereoselective

RX(35) OF 37 - 4 STEPS



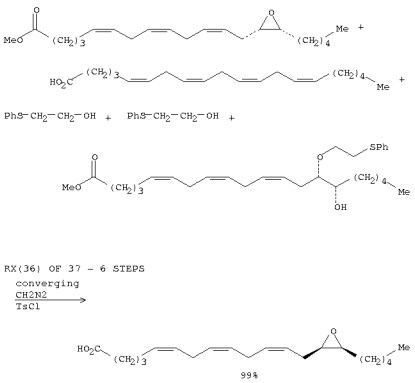
L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(35) OF 37 - 4 STEPS



NOTE: 58% overall yield, stereoselective, buffered soln., stereoselective, 76% overall yield, stereoselective

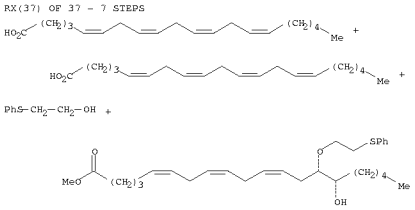
RX(36) OF 37 - 6 STEPS



NOTE: buffered soln., stereoselective, 76% overall yield, stereoselective, 58% overall yield, stereoselective, 76% overall yield, stereoselective

L26 ANSWER 13 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(37) OF 37 - 7 STEPS

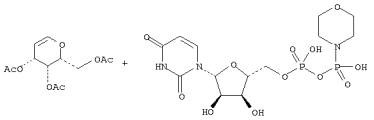


NOTE: buffered soln., stereoselective, 76% overall yield, stereoselective, 58% overall yield, stereoselective, buffered soln., stereoselective, 76% overall yield, stereoselective

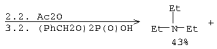
RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 14 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 135:192086 CASREACT
TI Mechanistic Investigation of UDP-Galactopyranose Mutase from Escherichia coli Using 2- and 3-Fluorinated UDP-Galactofuranose as Probes
AU Zhang, Qibo; Liu, Hung-wen
CS Division of Medicinal Chemistry College of Pharmacy and Department of Chemistry and Biochemistry, University of Texas, Austin, TX, 78712, USA
SO Journal of the American Chemical Society (2001), 123(28), 6756-6766
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB The galactofuranose moiety found in many surface constituents of microorganisms is derived from UDP-D-galactopyranose (UDP-Galp) via a unique ring contraction reaction catalyzed by UDP-Galp mutase. This enzyme, which has been isolated from several bacterial sources, is a flavoprotein. To study this catalysis, the cloned Escherichia coli mutase was purified and two fluorinated analogs, UDP-[2-F]Galf (9) and UDP-[3-F]Galf (10), were chemical synthesized. These two compds. were found to be substrates for the reduced UDP-Galp mutase with the Km values determined to be 65 and 861 μM for 9 and 10, resp., and the corresponding kcat values estimated to be 0.033 and 5.7 s-1. Since the fluorine substituent is redox inert, a mechanism initiated by the oxidation of 2-OH or 3-OH on the galactose moiety can thus be firmly ruled out. Furthermore, both 9 and 10 are poorer substrates than UDP-Galf, and the rate reduction for 9 is especially significant. This finding may be ascribed to the inductive effect of the 2-F substituent that is immediately adjacent to the anomeric center, and is consistent with a mechanism involving formation of oxocarbenium intermediates or transition states during turnover. Interestingly, under nonreducing conditions, compds. 9 and 10 are not substrates, but instead are inhibitors for the mutase. The inactivation by 10 is time-dependent, active-site-directed, and irreversible with a KI of 270 μM and a kinact of 0.19 min-1. Since the KI value is similar to Km, the observed inactivation is unlikely a result of tight binding. To our surprise, the inactivated enzyme could be regenerated in the presence of dithionite, and the reduced enzyme is resistant to inactivation by these fluorinated analogs. It is possible that reduction of the enzyme-bound FAD may induce a conformational change that facilitates the breakdown of the putative covalent enzyme-inhibitor adduct to reactivate the enzyme. It is also conceivable that the reduced flavin bears a higher electron d. at N-1, which may play a role in preventing the formation of the covalent adduct or facilitating its breakdown by charge stabilization of the oxocarbenium intermediates/transition states. Clearly, this study has led to the identification of a potent inactivator (10) for this enzyme, and study of its inactivation has also shed light on the possible mechanism of this mutase.

RX(60) OF 84 - 6 STEPS



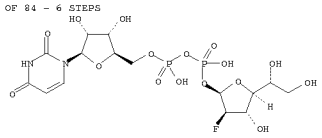
(step 6)



43%

L26 ANSWER 14 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

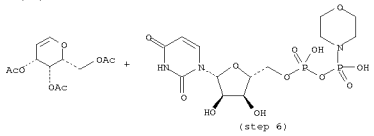
RX(60) OF 84 - 6 STEPS



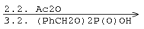
43%

NOTE: 2) key step, stereoselective, 3) stereoselective

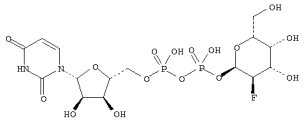
RX(63) OF 84 - 7 STEPS



(step 6)



RX(63) OF 84 - 7 STEPS



NOTE: 2) key step, stereoselective, 3) stereoselective, 7) buffered soln., biotransformation, mutase used

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 15 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 133:208175 CASREACT
TI Chemoenzymatic synthesis of PSGL-1 glycopeptides: sulfation on tyrosine affects glycosyltransferase-catalyzed synthesis of the O-glycan
AU Koeller, K. M.; Smith, M. E. B.; Wong, C.-H.
CS Department of Chemistry, The Scripps Research Institute and Skaggs Institute for Chemical Biology, La Jolla, CA, 92037, USA
SO Bioorganic & Medicinal Chemistry (2000), 8(5), 1017-1025
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
AB P-selectin glycoprotein ligand-1 (PSGL-1) is the primary glycoprotein ligand for P-selectin during the inflammatory response. Interestingly, the N-terminal sequence, containing both a site of tyrosine sulfation and an O-glycan, has been shown to bind to P-selectin with an affinity similar to full-length PSGL-1. To further characterize this system, the synthesis of glycopeptides from PSGL-1 was undertaken. The synthesis involved both solution- and solid-phase synthesis, as well as enzymic transformations. During the synthesis, notable reactivity differences of the glycosyltransferases toward sulfated and unsulfated versions of the same glycopeptides were observed

RX(10) OF 41 - REACTION DIAGRAM NOT AVAILABLE

RX(11) OF 41 - REACTION DIAGRAM NOT AVAILABLE

RX(12) OF 41 - REACTION DIAGRAM NOT AVAILABLE

RX(19) OF 41 - REACTION DIAGRAM NOT AVAILABLE

RX(20) OF 41 - REACTION DIAGRAM NOT AVAILABLE

RX(22) OF 41 - REACTION DIAGRAM NOT AVAILABLE

RX(23) OF 41 - REACTION DIAGRAM NOT AVAILABLE

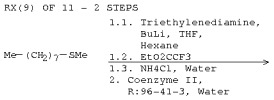
RX(31) OF 41 - REACTION DIAGRAM NOT AVAILABLE

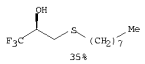
RX(34) OF 41 - REACTION DIAGRAM NOT AVAILABLE

RX(35) OF 41 - REACTION DIAGRAM NOT AVAILABLE
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 16 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 129:188889 CASREACT
TI Asymmetric reduction of trifluoromethyl ketones containing a sulfur functionality by the alcohol dehydrogenase from Geotrichum
AU Nakamura, Kaoru; Matsuda, Tomoko; Shimizu, Makoto; Fujisawa, Tamotsu
CS Institute for Chemical Research, Kyoto University, Kyoto, 611, Japan
SO Tetrahedron (1998), 54(29), 8393-8402
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
AB The reduction of trifluoromethyl ketones containing a S functionality by the crude alc. dehydrogenase from Geotrichum proceeded successfully, and the corresponding optically active alcs. were synthesized with high yields and excellent enantioselectivities.

RX(9) OF 11 - 2 STEPS





35%

NOTE: 2) stereoselective, enzymic, biotransformation, acetone powder of Geotrichum candidum IFO4597 (APG4 system) containing alcohol dehydrogenase used, MES buffered solution used, ee > 95%
CON: STEP(1.1) -20 deg C; 3 hours, 0 deg C
STEP(1.2) -78 deg C; 3 hours, -78 deg C
STEP(2) 18 hours, 30 deg C, pH 7

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 17 OF 25 CASREACT COPYRIGHT 2008 ACS on STN

AN 126:58943 CASREACT

TI Quantitative conversion of indene to (1S,2R) indene oxide and (1S,2R)-indanediol by combination of haloperoxidase bioconversion and chemical steps

IN Chartrain, Michel M.; Connors, Neal C.; Garrity, George M.; Olewinski, Roger C., Jr.; Verhoeven, Thomas R.; Zhang, Jinyou

PA Merck and Co., Inc., USA

SO PCT Int. Appl., 53 pp.
CODEN: PIXXD2

DT Patent

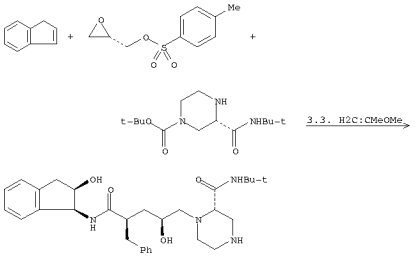
LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO-----9636724	A1	19961121	1996WO-US0006954	19960515
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US-----5605819	A	19970225	1995US-000445154	19950519
AU-----9657497	A	19961129	1996AU-000057497	19960515
CN-----1190994	A	19980819	1996CN-000195618	19960515
CN-----1066772	B	20010606		
BR-----9608720	A	19990629	1996BR-000008720	19960515
PRAI 1995US-000445154		19950519		
1996WO-US0006954		19960515		

AB A process is disclosed that quant. bioconverts indene to (1S,2R)-indene oxide and (1S,2R)-indanediol by the action of fungal haloperoxidase followed by various chemical step(s), e.g., adjusting the pH.

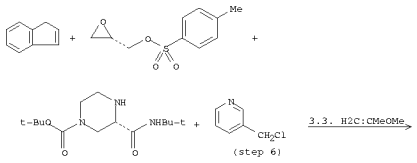
RX(46) OF 89 - 5 STEPS



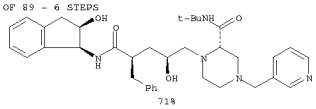
NOTE: 1) buffered soln. pH 10.5

L26 ANSWER 17 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(51) OF 89 - 6 STEPS

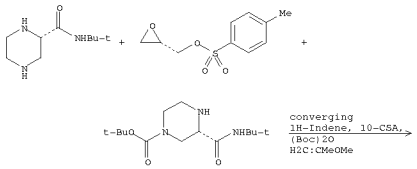


RX(51) OF 89 - 6 STEPS

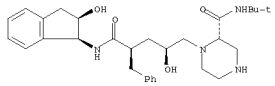


NOTE: 1) buffered soln. pH 10.5

RX(52) OF 89 - 6 STEPS



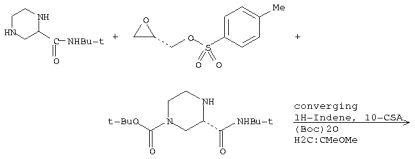
RX(52) OF 89 - 6 STEPS



NOTE: buffered soln. pH 10.5

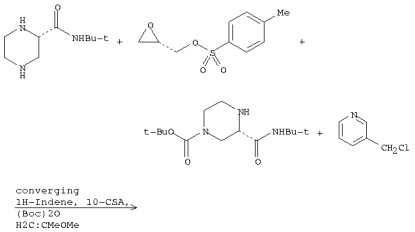
L26 ANSWER 17 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(56) OF 89 - 7 STEPS

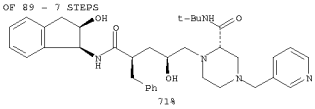


NOTE: buffered soln. pH 10.5, stereoselective, resoln. step

RX(69) OF 89 - 7 STEPS



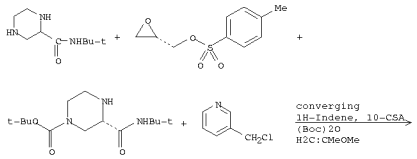
RX(69) OF 89 - 7 STEPS



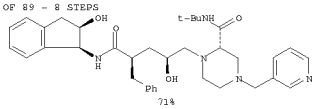
NOTE: buffered soln. pH 10.5

L26 ANSWER 17 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(70) OF 89 - 8 STEPS

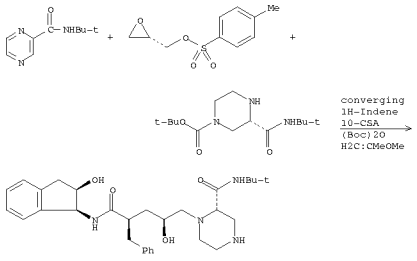


RX(70) OF 89 - 8 STEPS



NOTE: buffered soln. pH 10.5, stereoselective, resoln. step

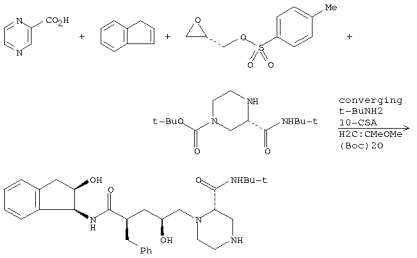
RX(71) OF 89 - 8 STEPS



NOTE: buffered soln. pH 10.5, catalyst on carbon, solid-supported catalyst, stereoselective, resoln. step

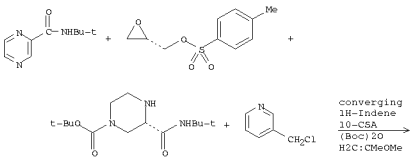
L26 ANSWER 17 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(83) OF 89 - 9 STEPS

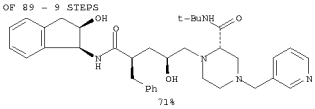


NOTE: buffered soln. pH 10.5, catalyst on carbon, solid-supported catalyst, stereoselective, resoln. step

RX(88) OF 89 - 9 STEPS



RX(88) OF 89 - 9 STEPS

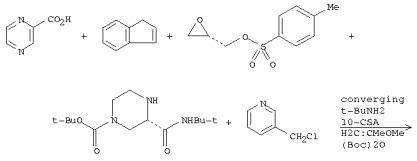


71%

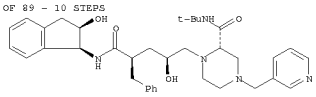
NOTE: buffered soln. pH 10.5, catalyst on carbon, solid-supported catalyst, stereoselective, resoln. step

L26 ANSWER 17 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(89) OF 89 - 10 STEPS



RX(89) OF 89 - 10 STEPS



71%

NOTE: buffered soln. pH 10.5, catalyst on carbon, solid-supported catalyst, stereoselective, resoln. step

L26 ANSWER 18 OF 25 CASREACT COPYRIGHT 2008 ACS on STN

AN 115:159542 CASREACT

TI Enzymic synthesis of β-D-glucuronides with in situ regeneration of uridine 5'-diphosphoglucuronic acid

AU Gygax, Daniel; Spies, Peter; Winkler, Tammo; Pfaar, Ulrike

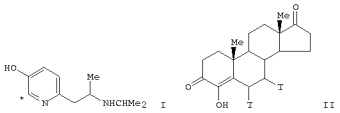
CS Pharm. Div., Ciba-Geigy Ltd., Basel, CH-4002, Switz.

SO Tetrahedron (1991), 47(28), 5119-22
CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

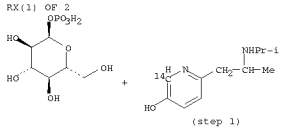
GI



I II

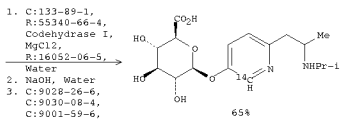
AB β-D-Glucuronides of I and II were synthesized by a multi-enzyme system with in situ regeneration of uridine 5'-diphosphoglucuronic acid. Crude liver homogenate containing all enzymes involved in the multi-enzyme system was used for this stereoselective one-pot reaction.

RX(1) OF 2



2 Na

(step 1)



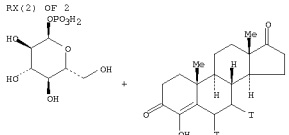
(step 1)

65%

NOTE: enzymic; crude guinea pig liver homogenate; pH 8.0

L26 ANSWER 18 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

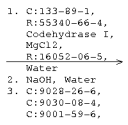
RX(2) OF 2



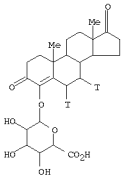
2 Na

(step 1)

(step 1)



RX(2) OF 2



28%

NOTE: enzymic; crude rabbit liver homogenate; pH 8.0

L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN

AN 113:6687 CASREACT

TI Fluorinated analogs of Ins(1,4,5)P3

AU Marecek, James F.; Prestwich, Glenn D.

CS Dep. Chem., State Univ. New York, Stony Brook, NY, 11794-3400, USA

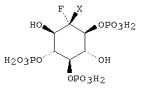
SO Tetrahedron Letters (1989), 30(40), 5401-4

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

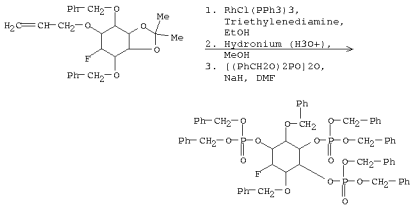
GI



I

AB 2-Fluoro-2-deoxy-Ins(1,4,5)P3 (I; X = H) and 2,2-difluoro-2-deoxy-Ins(1,4,5)P3, I (X = F), were synthesized from protected inositol precursors. The monofluoro compound with free 3,6-hydroxyl groups underwent slow defluorination at pH >13, as determined by 19F NMR, while the difluoro compound was inert.

RX(33) OF 52 - 3 STEPS



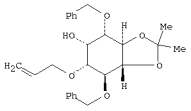
1. RhCl(PPh3)3, Triethylenediamine, EtOH
2. Hydronium (H3O+), MeOH
3. [(PhCH2O)2PO]2O, NaH, DMF

44%

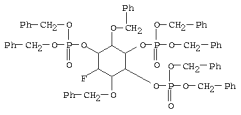
NOTE: 1) 91% overall, 2) 83% overall

L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(34) OF 52 - 4 STEPS



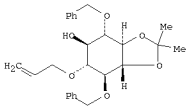
1. DAST [(Et2N).SF3], CH2Cl2
2. RhCl(PPh3)3, Triethylenediamine, EtOH
3. Hydronium (H3O+), MeOH
4. [(PhCH2O)2PO]2O, NaH, DMF



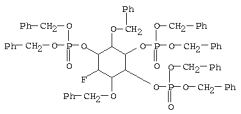
44%

NOTE: 2) 91% overall, 3) 83% overall

RX(35) OF 52 - 4 STEPS



1. DAST [(Et2N).SF3], CH2Cl2
2. RhCl(PPh3)3, Triethylenediamine, EtOH
3. Hydronium (H3O+), MeOH
4. [(PhCH2O)2PO]2O, NaH, DMF

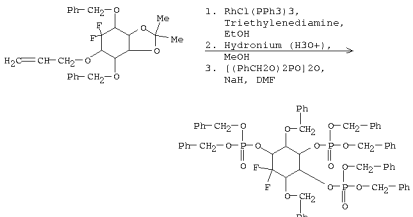


44%

NOTE: 2) 91% overall, 3) 83% overall

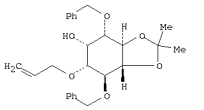
L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(36) OF 52 - 3 STEPS

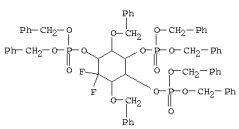


1. RhCl(PPh3)3, Triethylenediamine, EtOH
2. Hydronium (H3O+), MeOH
3. [(PhCH2O)2PO]2O, NaH, DMF

RX(37) OF 52 - 4 STEPS

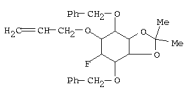


1. DAST [(Et2N).SF3], CH2Cl2
2. RhCl(PPh3)3, Triethylenediamine, EtOH
3. Hydronium (H3O+), MeOH
4. [(PhCH2O)2PO]2O, NaH, DMF

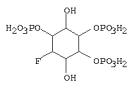


L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(39) OF 52 - 4 STEPS



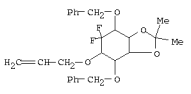
1. RhCl(PPh3)3, Triethylenediamine, EtOH
2. Hydronium (H3O+), MeOH
3. [(PhCH2O)2PO]2O, NaH, DMF
4. Pd, H2, EtOH



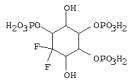
6 Na

NOTE: 1) 91% overall, 2) 83% overall

RX(41) OF 52 - 4 STEPS



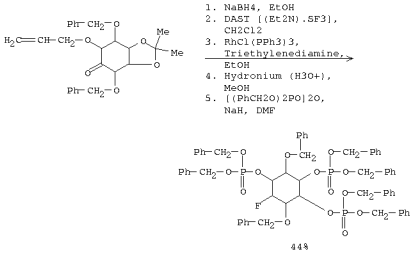
1. RhCl(PPh3)3, Triethylenediamine, EtOH
2. Hydronium (H3O+), MeOH
3. [(PhCH2O)2PO]2O, NaH, DMF
4. Pd, H2, EtOH



6 Na

L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

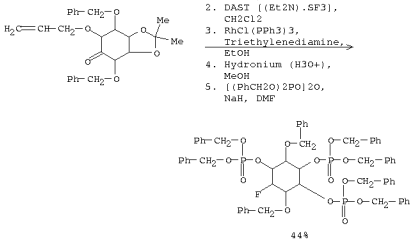
RX(44) OF 52 - 5 STEPS



44%

NOTE: 3) 91% overall, 4) 83% overall

RX(45) OF 52 - 5 STEPS

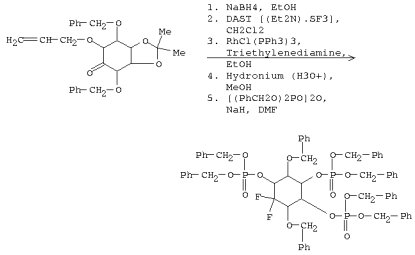


44%

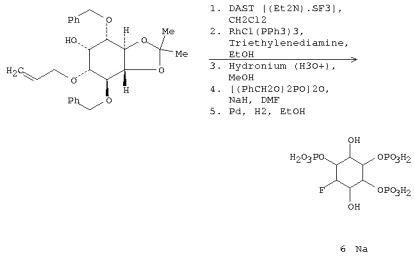
NOTE: 3) 91% overall, 4) 83% overall

L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(46) OF 52 - 5 STEPS



RX(47) OF 52 - 5 STEPS

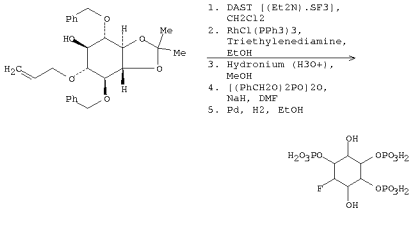


6 Na

NOTE: 2) 91% overall, 3) 83% overall

L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

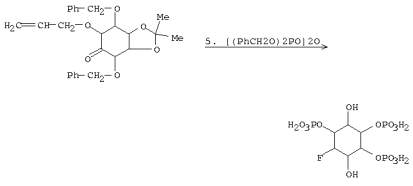
RX(48) OF 52 - 5 STEPS



6 Na

NOTE: 2) 91% overall, 3) 83% overall

RX(49) OF 52 - 6 STEPS

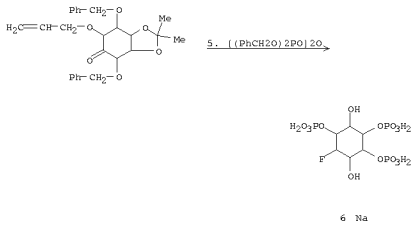


6 Na

NOTE: 3) 91% overall, 4) 83% overall

L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

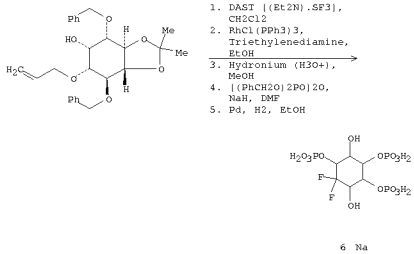
RX(50) OF 52 - 6 STEPS



6 Na

NOTE: 3) 91% overall, 4) 83% overall

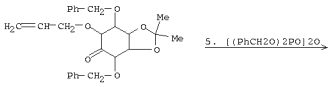
RX(51) OF 52 - 5 STEPS

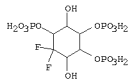


6 Na

L26 ANSWER 19 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

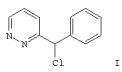
RX(52) OF 52 - 6 STEPS





6 Na

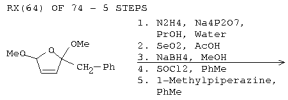
L26 ANSWER 20 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 113:6262 CASREACT
TI Pyridazines. L. Syntheses and reactions of phenyl(3-pyridazinyl)methane derivatives
AU Heinisch, Gottfried; Huber, Thierry
CS Inst. Pharm. Chem., Univ. Vienna, Vienna, A-1090, Austria
SO Journal of Heterocyclic Chemistry (1989), 26(6), 1787-91
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
GI

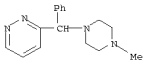


I

AB A convenient approach to phenyl 3-pyridazinyl ketone and phenyl(3-pyridazinyl)methanol is proposed. Reactions of the related diarylmethyl chloride with various N- and S-nucleophiles were found to afford the expected amines and thioethers in satisfactory yields.

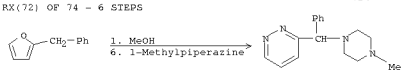
RX(64) OF 74 - 5 STEPS





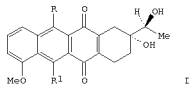
73%

RX(72) OF 74 - 6 STEPS

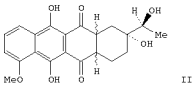


73%

L26 ANSWER 21 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 112:178434 CASREACT
TI Reductive transformations of 10-deoxydaunomycinone
AU Brand, David J.; Fisher, Jed F.
CS Dep. Chem., Univ. Minnesota, Minneapolis, MN, 55455, USA
SO Journal of Organic Chemistry (1990), 55(8), 2518-30
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
GI



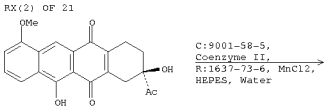
I

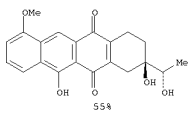


II

AB An enzyme system consisting of spinach ferredoxin-NADP+ reductase, pig heart isocitric dehydrogenase (NADP+), spinach ferredoxin, and either of the coenzymes NAD(P)H reduced an aqueous anaerobic solution of daunomycin and gave two tetrahyrodihydroxynaphthacenediones I (R = HO, R1 = H; R = H, R1 = HO) and three diastereomers of hexahydrotrihydroxynaphthacenedione II that differ in stereochem. at the C-4a,C-12a ring juncture. Virtually identical results were observed when either daunomycinone or (1'S)-1'-dihydrodaunomycinone, instead of daunomycin, were used as a substrate for the enzyme system. However, a different set of products, epimeric to those formed when (1'S)-1'-dihydrodaunomycinone was the substrate, were produced when (1'R)-1'-dihydrodaunomycinone was used. All of these products had the R configuration at the C(1') stereogenic center.

RX(2) OF 21



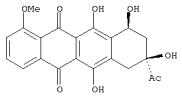


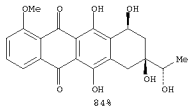
55%

NOTE: pH 7.0 buffer

L26 ANSWER 21 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(3) OF 21

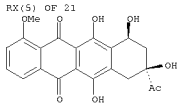




84%

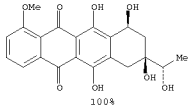
NOTE: pH 7.0 buffer

RX(5) OF 21



(step 1)

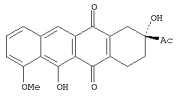
1. MnCl2, Coenzyme II, R:1637-73-6, HEPES, D-Glucose, DMF, Water
2. C:9001-58-5, C:9001-37-0, Catalase

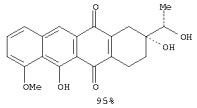


100%

NOTE: pH 7.0 buffer

RX(8) OF 21



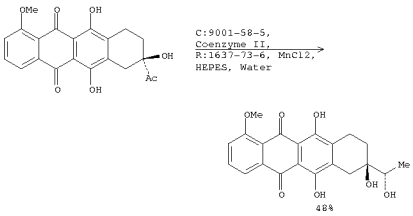


95%

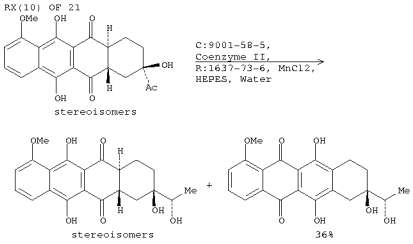
NOTE: pH 7.0 buffer

L26 ANSWER 21 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(9) OF 21



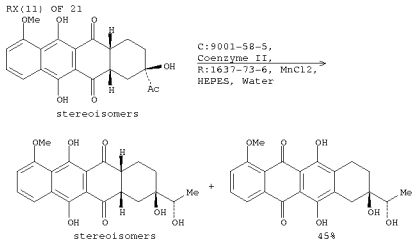
RX(10) OF 21



NOTE: pH 7.0 buffer

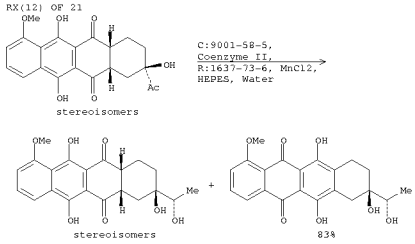
L26 ANSWER 21 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(11) OF 21



NOTE: pH 7.0 buffer

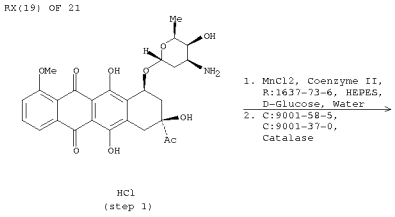
RX(12) OF 21



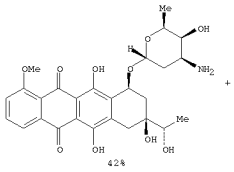
NOTE: pH 7.0 buffer

L26 ANSWER 21 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

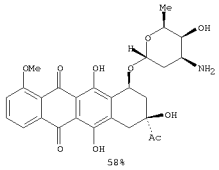
RX(19) OF 21



RX(19) OF 21



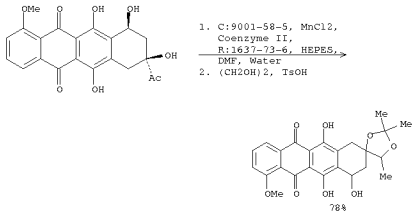
RX(19) OF 21



NOTE: pH 7.0 buffer

L26 ANSWER 21 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(20) OF 21 - 2 STEPS



NOTE: 1) pH 7.0 buffer, 2) sonication

L26 ANSWER 22 OF 25 CASREACT COPYRIGHT 2008 ACS on STN

AN 112:99044 CASREACT

TI The total synthesis of myo-inositol phosphates via myo-inositol orthoformate

AU Billington, David C.; Baker, Raymond; Kulagowski, Janusz J.; Mawer, Ian M.; Vacca, Joseph P.; DeSolms, S. Jane; Huff, Joel R.

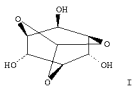
CS Neurosci. Res. Cent., Merck Sharp and Dohme Res. Lab., Harlow/Essex, CM20 2QR, UK

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1989), (8), 1423-9
CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

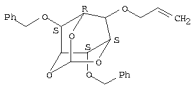
GI



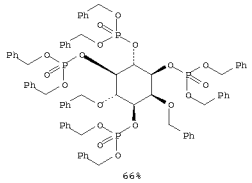
I

AB Novel selective alkylations of myo-inositol orthoformate (I) have been used to prepare a series of protected myo-inositol derivs. These intermediates have been used in efficient total syntheses of myo-inositol 2-phosphate, (II), myo-inositol 4-phosphate (III), myo-inositol 1,3-bisphosphate (IV), and myo-inositol 1,3,4,5-tetrakisphosphate (V). This report represents the first total synthesis of the important natural metabolites IV and V and significantly improved methods of preparation of II and III.

RX(31) OF 55 - 2 STEPS



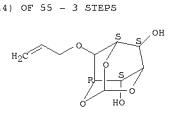
1.1. RhCl(PPh3)3, Triethylenediamine, Water, EtOH
1.2. HCl, MeOH
2.1. NaH, THF
2.2. [(PhCH2O)2PO]2O, 1H-Imidazole



66%

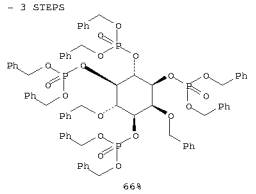
L26 ANSWER 22 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(44) OF 55 - 3 STEPS



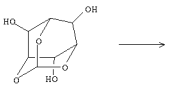
1.1. NaH, DMF
1.2. PhCH2Br
2.1. RhCl(PPh3)3, Triethylenediamine, Water, EtOH
2.2. HCl, MeOH
3.1. NaH, THF
3.2. [(PhCH2O)2PO]2O, 1H-Imidazole

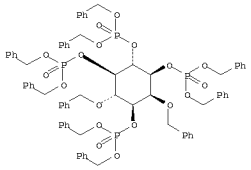
RX(44) OF 55 - 3 STEPS



66%

RX(45) OF 55 - 4 STEPS

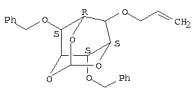




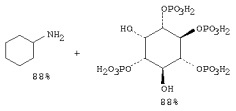
66%

L26 ANSWER 22 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(46) OF 55 - 3 STEPS



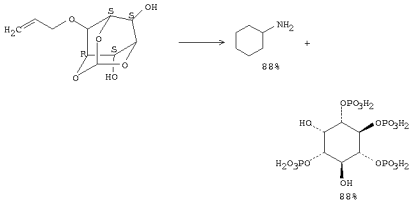
1.1. RhCl(PPh3)3, Triethylenediamine, Water, EtOH
1.2. HCl, MeOH
2.1. NaH, THF
2.2. [(PhCH2O)2PO]2O, 1H-Imidazole
3.1. Pd, H2, Water, EtOH
3.2. Cyclohexylamine



88%

88%

RX(47) OF 55 - 4 STEPS

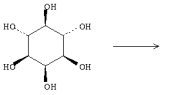


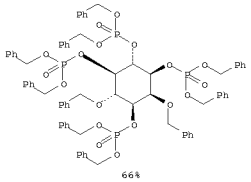
88%

88%

L26 ANSWER 22 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

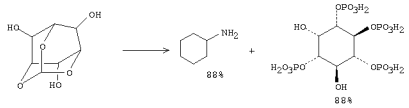
RX(52) OF 55 - 5 STEPS





66%

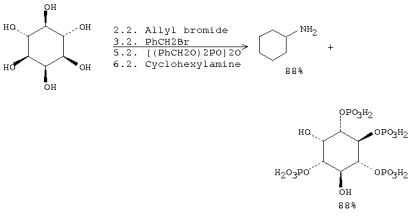
RX(54) OF 55 - 5 STEPS



88%

88%

RX(55) OF 55 - 6 STEPS



2.2. Allyl bromide
3.2. PhCH2Br
5.2. [(PhCH2O)2PO]2O
6.2. Cyclohexylamine

88%

88%

L26 ANSWER 23 OF 25 CASREACT COPYRIGHT 2008 ACS on STN

AN 111:134090 CASREACT

TI Sterically hindered 5,11-dicarbo analogs of clozapine as potential chiral antipsychotic agents

AU Rupard, J. Howard; De Paulis, Tomas; Janowsky, Aaron; Smith, Howard E.

CS Dep. Chem., Vanderbilt Univ., Nashville, TN, 37235, USA

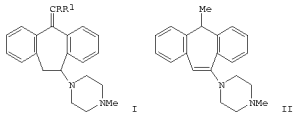
SO Journal of Medicinal Chemistry (1989), 32(10), 2261-8

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

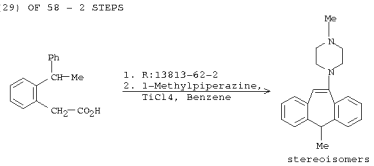
GI



I II

AB Title compds. I (R = R1 = H, Me; R = H, R1 = Me) and II were prepared NMR studies showed that I (R = R1 = H) exists at room temperature as configurational enantiomers, but the activation energy for thermal racemization is 19 kcal mol-1 at 105°, and it is doubtful that the enantiomers can be isolated under usual laboratory conditions. (Z)-I (R = H, R1 = Me) and I (R = R1 = Me) have activation energies >23 kcal mol-1 at 160°, and there is a possibility that they can be obtained as their resp. enantiomers. II incorporates a chiral center which is not thermally racemized, but it exists at room temperature as two diastereomers with an activation energy for inversion of the dibenzocycloheptene ring of 21 kcal mol-1. When I and II were tested in vitro for biol. activity, their affinities for muscarinic and dopamine D-1 and D-2 sites were lower than that of clozapine but were still substantial. Thus, the resp. biol. activities of the racemates indicate that the biol. activities of the thermally stable enantiomers may be of importance in finding a clozapine derivative with fewer side effects than those shown by clozapine itself. Because of the susceptibility of the enamines to acid-catalyzed hydrolysis, resolution into resp. enantiomers is not anticipated.

RX(29) OF 58 - 2 STEPS

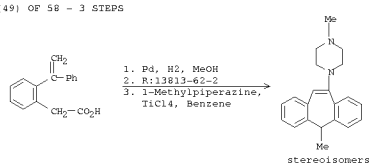


stereoisomers

NOTE: 1) 64% overall yield, 2) 55% overall yield; 4:1 diastereomer ratio

L26 ANSWER 23 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

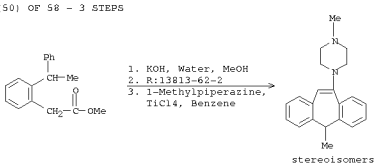
RX(49) OF 58 - 3 STEPS



stereoisomers

NOTE: 2) 64% overall yield, 3) 55% overall yield; 4:1 diastereomer ratio

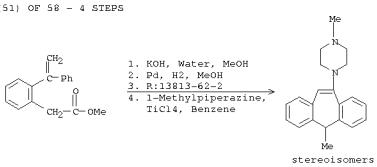
RX(50) OF 58 - 3 STEPS



stereoisomers

NOTE: 2) 64% overall yield, 3) 55% overall yield; 4:1 diastereomer ratio

RX(51) OF 58 - 4 STEPS

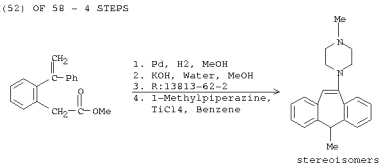


stereoisomers

NOTE: 3) 64% overall yield, 4) 55% overall yield; 4:1 diastereomer ratio

L26 ANSWER 23 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

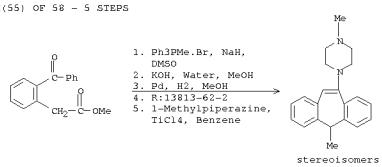
RX(52) OF 58 - 4 STEPS



stereoisomers

NOTE: 3) 64% overall yield, 4) 55% overall yield; 4:1 diastereomer ratio

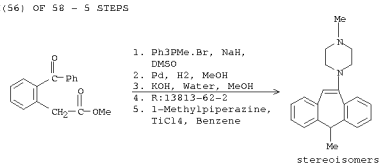
RX(55) OF 58 - 5 STEPS



stereoisomers

NOTE: 4) 64% overall yield, 5) 55% overall yield; 4:1 diastereomer ratio

RX(56) OF 58 - 5 STEPS

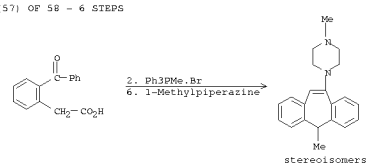


stereoisomers

NOTE: 4) 64% overall yield, 5) 55% overall yield; 4:1 diastereomer ratio

L26 ANSWER 23 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

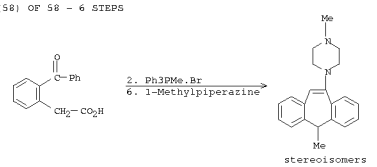
RX(57) OF 58 - 6 STEPS



stereoisomers

NOTE: 5) 64% overall yield, 6) 55% overall yield; 4:1 diastereomer ratio

RX(58) OF 58 - 6 STEPS

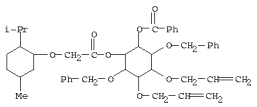


stereoisomers

NOTE: 5) 64% overall yield, 6) 55% overall yield; 4:1 diastereomer ratio

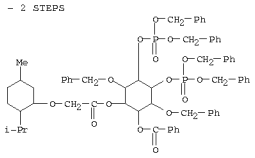
L26 ANSWER 24 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 110:173629 CASREACT
TI A versatile intermediate, D-4,5-bis(dibenzyl phosphoryl)-myo-inositol derivative, for synthesis of inositol phosphates. Synthesis of 1,2-cyclic-4,5-, 1,4,5-, and 2,4,5-trisphosphate
AU Watanabe, Yutaka; Ogasawara, Tomio; Nakahira, Hiroyuki; Matsuki, Tomoko; Ozaki, Shoichiro
CS Fac. Eng., Ehime Univ., Matsuyama, 790, Japan
SO Tetrahedron Letters (1988), 29(41), 5259-62
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
AB D-myo-Inositol 1,2-cyclic-4,5-, 1,4,5-, and 2,4,5-trisphosphate were prepared from the key synthetic intermediate, D-3,6-di-O-benzyl-4,5-di-O-(dibenzyl phosphoryl)-myo-inositol, which was prepared from myo-inositol in 5 steps.

RX(18) OF 52 - 2 STEPS



1.1. RhCl(PPh3)3, Triethylenediamine
1.2. HCl, MeOH
2. [(PhCH2O)2PO]2O, BuLi

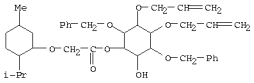
RX(18) OF 52 - 2 STEPS



70%

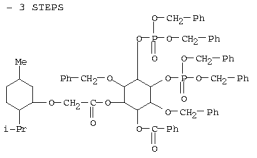
L26 ANSWER 24 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(29) OF 52 - 3 STEPS



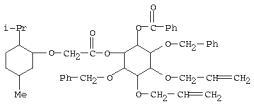
1. PhCOCl, Pyridine
2.1. RhCl(PPh3)3, Triethylenediamine
2.2. HCl, MeOH
3. [(PhCH2O)2PO]2O, BuLi

RX(29) OF 52 - 3 STEPS

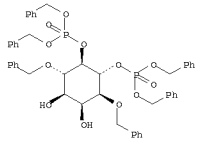


70%

RX(30) OF 52 - 3 STEPS



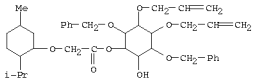
1.1. RhCl(PPh3)3, Triethylenediamine
1.2. HCl, MeOH
2. [(PhCH2O)2PO]2O, BuLi
3. NH3, MeOH



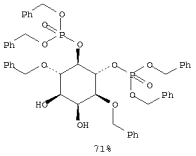
71%

L26 ANSWER 24 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(31) OF 52 - 4 STEPS



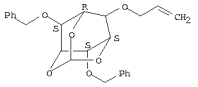
1. PhCOCl, Pyridine
2.1. RhCl(PPh3)3, Triethylenediamine
2.2. HCl, MeOH
3. [(PhCH2O)2PO]2O, BuLi
4. NH3, MeOH



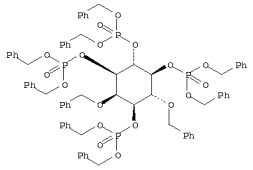
71%

L26 ANSWER 25 OF 25 CASREACT COPYRIGHT 2008 ACS on STN
AN 109:6847 CASREACT
TI Synthesis of myo-inositol 1,3,4,5-tetraphosphate and myo-inositol 1,3-bisphosphate
AU Billington, David C.; Baker, Raymond
CS Neurosci. Res. Cent., Merck Sharp and Dohme Res. Lab., Harlow/Essex, CM20 2QR, UK
SO Journal of the Chemical Society, Chemical Communications (1987), (13), 1013-13
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB myo-Inositol 1,3,4,5-tetraphosphate (I), myo-inositol 1,3-diphosphate, and myo-inositol 4-phosphate were prepared via routes in which a key step was a novel, highly regioselective O-monoalkylation of myo-inositol orthoformate (II).

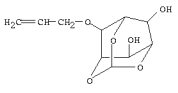
RX(14) OF 28 - 2 STEPS



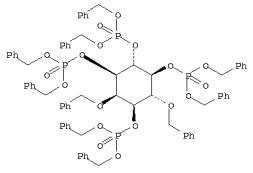
1.1. RhCl(PPh3)3, Triethylenediamine, EtOH
1.2. HCl, MeOH
2. [(PhCH2O)2PO]2O, NaH, 1H-Imidazole, THF



RX(21) OF 28 - 3 STEPS

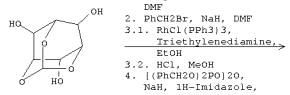


1. PhCH2Br, NaH, DMF
2.1. RhCl(PPh3)3, Triethylenediamine, EtOH
2.2. HCl, MeOH
3. [(PhCH2O)2PO]2O, NaH, 1H-Imidazole, THF



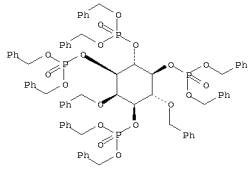
L26 ANSWER 25 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(22) OF 28 - 4 STEPS

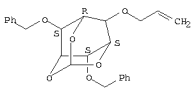


1. Allyl bromide, NaH, DMF
2. PhCH2Br, NaH, DMF
3.1. RhCl(PPh3)3, Triethylenediamine, EtOH
3.2. HCl, MeOH
4. [(PhCH2O)2PO]2O, NaH, 1H-Imidazole, THF

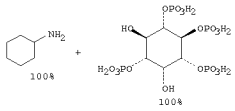
RX(22) OF 28 - 4 STEPS



RX(23) OF 28 - 3 STEPS



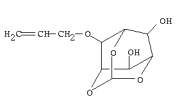
1.1. RhCl(PPh3)3, Triethylenediamine, EtOH
1.2. HCl, MeOH
2. [(PhCH2O)2PO]2O, NaH, 1H-Imidazole, THF
3. Pd, H2, EtOH, Water



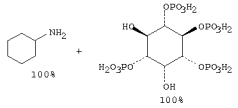
100% 100%

L26 ANSWER 25 OF 25 CASREACT COPYRIGHT 2008 ACS on STN (Continued)

RX(24) OF 28 - 4 STEPS

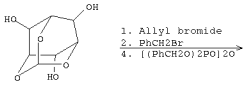


1. PhCH2Br, NaH, DMF
2.1. RhCl(PPh3)3, Triethylenediamine, EtOH
2.2. HCl, MeOH
3. [(PhCH2O)2PO]2O, NaH, 1H-Imidazole, THF
4. Pd, H2, EtOH, Water



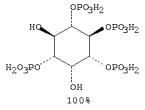
100% 100%

RX(28) OF 28 - 5 STEPS



1. Allyl bromide
2. PhCH2Br
4. [(PhCH2O)2PO]2O

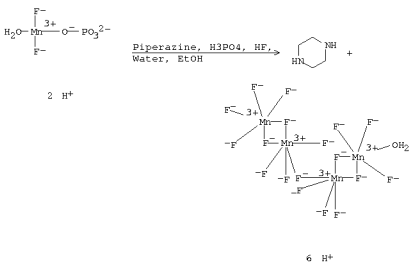
100%



=> d bib abs crd l18 tot

L18 ANSWER 1 OF 3 CASREACT COPYRIGHT 2008 ACS on STN
AN 142:384442 CASREACT
TI Fluoromanganate(III) anions with new tetrameric and chain structures in (pipzH2)3[Mn4F18(H2O)].(H2O) and (pipzH2)4[Mn2F3]2[MnF4(H2O)2][MnF4(HF)2]
AU Stief, Ronald; Massa, Werner
CS Fachbereich Chemie, Philipps-Universitaet Marburg, Marburg, D-35032, Germany
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (2004), 630(13-14), 2502-2507
CODEN: ZAACAB; ISSN: 0044-2313
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA German
AB In the course of systematic investigations of pptns. from hydrofluoric acid solns. of Mn(III) and piperazine, the both title compds., (pipzH2)3[Mn4F18(H2O)].(H2O) and (pipzH2)4[Mn2F3]2[MnF4(H2O)2][MnF4(HF)2], were obtained and characterized by x-ray crystallog. (pipzH2)3[Mn4F18(H2O)].(H2O) crystallizes in the orthorhombic system, space group Pnma, Z = 4, a = 2050.8(2), b = 1253.0(1), c = 1096.0(1) pm, dc = 2.034, 2894 observed reflections with I > 2σ(I), 298 refined parameters, R1 = 0.0290, wR2 = 0.0568. The structure shows a new tetrameric anion [Mn4F18(H2O)]6- composed by 2 edge-sharing double-octahedra linked by a common corner. (pipzH2)4[Mn2F9]2[MnF4(H2O)2][MnF4(HF)2] is triclinic, space group P.hivin.1, Z = 1, a = 901.6(1), b = 913.1(1), c = 1308.9(1) pm, α = 70.024(6)°, β = 75.229(6)°, γ = 78.887(6)°, dc = 2.138, 3240 observed reflections with I > 2σ(I), 313 refined parameters, R1 = 0.0261, wR2 = 0.0544. Here, analogous double-octahedra with F ligands only are corner-linked to infinite chains. These are further connected by strong H-bonds F···H···F, O···H···F, and N···H···F via isolated octahedral units [MnF4(H2O)2]- and [MnF4(HF)2]- as well as over the (pipzH2)2+ cations to form a 3D network. Typical for both structures, strong octahedral elongation is observed due to the Jahn-Teller effect. The long axes show parallel orientation within the plane of the double-bridging, both Mn-F-Mn bridges are strongly asym., therefore. Nevertheless, the ordering between the dimers is ferro-distortive in the tetramer but antiferro-distortive in the chain anion.

RX(1) OF 2



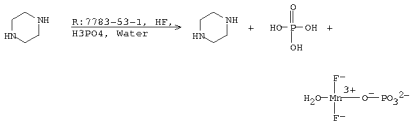
CON: 8 days, room temperature

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD

L18 ANSWER 1 OF 3 CASREACT COPYRIGHT 2008 ACS on STN (Continued)
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 3 CASREACT COPYRIGHT 2008 ACS on STN
AN 142:168235 CASREACT
TI Double-chain structure of (pipzH2)[MnF2(HPO4)(H2O)](H2PO4)
AU Stief, Ronald; Massa, Werner
CS Fachbereich Chemie and Wissenschaftliches Zentrum fuer Materialwissenschaften, Philipps-Universitaet Marburg, Marburg, D-35032, Germany
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (2004), 630(10), 1459-1461
CODEN: ZAACAB; ISSN: 0044-2313
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA German
AB By adding piperazine to a HF and H3PO4 solution of MnF3, the fluoride phosphate (pipzH2)[MnF2(HPO4)(H2O)](H2PO4) can be crystallized Its structure is built by piperazinium(2+) cations, (H2PO4)- anions, and an anionic double-chain of [HPO4] tetrahedra and [MnO3F2(H2O)] octahedra. The structure is triclinic, space qroup P.hivin.1, Z = 2, a = 622.97(4), b = 923.46(6), c = 1183 62(7) pm, α = 98.343(6)°, β = 100.747(7)°, γ = 107.642(5)°, dc = 2.092, 3061 observed reflections with I > 2σ(I), 250 refined parameters, R = 0.0289, wR2 = 0.0667. It is worth noting that a ferrodistortive Jahn-Teller order is observed with [MnO3F2(H2O)] octahedra strongly elongated along the F-Mn-OH2 axes perpendicular to the chain plane. The structure is stabilized by very strong H-bonds.

RX(1) OF 1

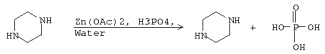


CON: 12 days, room temperature

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 3 CASREACT COPYRIGHT 2008 ACS on STN
AN 140:86413 CASREACT
TI Synthesis and characterization of [C4N2H12]1.5[Zn2(PO4)(HPO4)2]·H2O
AU Xing, Yan; Ding, Hong; Li, Guang-Hua; Shi, Zhan; Liu, Yun-Ling; Pang, Wen-Qin
CS State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University, Changchun, 130023, Peop. Rep. China
SO Wuji Huaxue Xuebao (2003), 19(8), 853-856
CODEN: WHUXEO; ISSN: 1001-4861
PB Wuji Huaxue Xuebao Bianjibu
DT Journal
LA Chinese
AB Using THF and H2O as solvent, piperazine as a template, a novel two-dimensional layered Zn phosphate [C4N2H12]1.5[Zn2(PO4)(HPO4)2]·H2O was prepared solvothermally, and its structure is determined at 293 K by Siemens Smart 1000 CCD diffractometer monoclinic, space group P21/c, a 0.81244(3), b 2.61706(12), c 0.83775(3) nm, β 110.981(2)°, Z = 4, R = 0.0285, Rw = 0.0719. The structure consists of vertex-sharing ZnO4, HPO4, and PO4 tetrahedra, and double-protonated organic cations, which gave undulating 4-ring chains and 12-ring sheets. A network of H bonds involving both layer-to-layer and layer-to-amine interaction holds the phosphate layer together.

RX(1) OF 1



CON: STAGE(1) 1 hour, room temperature; 120 hours, 100 deg C

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     FILE 'HCAPLUS' ENTERED AT 11:01:15 ON 01 MAY 2008
L1            1 US20060167256/PN

     FILE 'REGISTRY' ENTERED AT 11:01:30 ON 01 MAY 2008

     FILE 'HCAPLUS' ENTERED AT 11:01:35 ON 01 MAY 2008
L2              TRA L1 1- RN :        3 TERMS

     FILE 'REGISTRY' ENTERED AT 11:01:35 ON 01 MAY 2008
L3            3 SEA L2

     FILE 'REGISTRY' ENTERED AT 11:02:40 ON 01 MAY 2008
L4         3656 C4H10N2 AND NC2NC2/ES
L5           53 L4 AND H3O4P
L6            7 L4 AND H4O7P2

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     FILE 'REGISTRY' ENTERED AT 11:04:03 ON 01 MAY 2008

     FILE 'HCAPLUS' ENTERED AT 11:04:47 ON 01 MAY 2008
L7           38 PIPERAZINE (4A) (?PYROPHOSPHATE? OR DIPHOSPHATE (1A) 1 (1A) 1)
L8           38 L6
L9           45 L7-8
L10         128 L5
L11           7 PIPERAZINE (1A) (DIPHOSPHATE OR PHOSPHATE (1A) 1 (1A)2)
L12         132 L10-11
L13          20 L12 (L) RACT+NT/RL
L14          11 L9 (L) PREP+NT/RL
L15           1 L13 AND L14

     FILE 'HCAOLD' ENTERED AT 11:08:44 ON 01 MAY 2008
L16           0 L12 AND L9

     FILE 'USPATFULL, USPATOLD, USPAT2' ENTERED AT 11:09:07 ON 01 MAY 2008
L17           9 L10 AND L8

     FILE 'CASREACT' ENTERED AT 11:09:56 ON 01 MAY 2008
L18           3 L5
L19           0 L6
L20             STR
L21           0 L20
L22             STR L20
L23           1 L22
L24          97 L22 FULL EXTEND
L25          38 L22 FULL
L26          25 L25 AND (PD<=20040827 OR AD<=20040827 OR PRD<=20040827)

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L27           1 L15 AND L1
                SET EXTEND OFF PERM

     FILE 'CASREACT' ENTERED AT 11:21:25 ON 01 MAY 2008
L28           0 L1

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